

Appendix B

ANALYSIS OF EMISSION CONTROL BY A CATALYTIC RECUPERATOR AND BY UPSTREAM MONOLITHS

INTRODUCTION

[REDACTED] using post turbine catalytic monoliths and catalytically active exhaust-side recuperator surfaces to remove hydrocarbon and carbon monoxide emissions from the Capstone turbogenerators. [REDACTED]

[REDACTED] This report represents the detailed analysis, calculations, results, and conclusions. Also attached are the MathSoft Mathcad™ 6+ documents comprising the analyses and an Excel 5.0 spreadsheet of the findings.

TRANSPORT AND KINETIC ANALYSIS OF THE RECUPERATOR AND MONOLITHS

The analysis of the conversion of heptene (C_7H_{14}), methane (CH_4), and carbon monoxide (CO), were completed for several configurations of a recuperator and honeycomb catalytic converters. The method used was a MATHCAD program, and the procedures were similar to the document sent to Capstone [REDACTED] (CAPSTONE.MCD.document).

The analyses consist of the following features (see printouts for CPSTONE5.MCD and CPSTONE6.MCD):

Gas Properties

- The properties of the gases used in the combustion mixture are described on pages 1-8.
- The gas compositions both for complete combustion air with fuel equivalence ratio 0.1 in moist (2 vol% water vapor) air, as specified in the problem statement, and also for an adiabatic temperature rise from 1000° to 1511_F using heptene are defined on page 2. The difference in properties between these two compositions is insignificant.
- Essential transport properties, such as the diffusivities of the added gases are determined on pages 3-4.
- Mixture properties such as viscosity, thermal conductivity, heat capacity, and various dimensionless transport numbers such as the Prandtl and Schmidt numbers are defined and calculated on pages 5-8.

Recuperator and Converter Dimensions and Operating Conditions

- The dimensions of the honeycomb sizes from 100 to 800 cells/in.² are defined on page 9 along with the size and dimensions of the recuperator and the upstream monolith converters.
- The five operating combustion conditions representing the different power level cases for the turbogenerator are specified on pages 9-10.
- The pressure drop for the 600 or 800 cells/in.² recuperator is determined on page 11, and the analysis of heat transfer within the recuperator is described on page 12.

Recuperator Performance

- Mass transfer rates to the wall of the recuperator (assuming very fast conversion kinetics at the wall) are described on pages 13-14 for all three added components (C₇H₁₄, CH₄, and CO). These calculations used average temperatures to determine an integrated formula for fuel conversion.
- An alternative form of conversion was developed by looking at local Nusselt number (modified for the square channel configuration). This analysis is described on pages 15 and 16. The two methods show good agreement for C₇H₁₄ conversion.
- Catalytic properties and functions are defined on pages 17-18, and the specific rate expression for oxidation of dilute CH₄ by supported palladium oxide (PdO) is described on page 19.
- Slow (in CPSTONE5.MCD and related to the rate of CH₄ oxidation) and moderate (in CPSTONE6.MCD and related to the rate of C₃H₆ oxidation) rate constants for C₇H₁₄ oxidation are described on p. 19.
- The performance of the recuperator for conversion with temperature-dependent mass transfer properties and specific catalytic rates for C₇H₁₄ and CH₄ are described on pages 20-21.

Performance of Upstream Monoliths

- The operating conditions for 200, 400, and 600 cells/in.² honeycombs is described on pages 22-25.
- The pressure drop for three honeycombs (200, 400, and 600 cells/in.²) is described on pages 22-23, and matched to the maximum specified conditions. From of these calculations, two honeycomb converter configurations, 400 cells/in.² by 4 in. length and 600 cells/in.² by 3.5 in. length, were chosen for mass transfer calculations.
- The effluent concentrations of added components are calculated for the constant temperature monoliths (400 cells/in.² in CPSTONE5.MCD and 600 cells/in.² in CPSTONE6.MCD) for the five operating conditions (cases) on pages 24-25, assuming very fast catalytic rates.
- Finally, on pages 25-27, the conversion of C₇H₁₄ and CH₄ using finite catalytic rates are described for the honeycomb converters (400 cells/in.² in CPSTONE5.MCD and 600 cells/in.² in CPSTONE6.MCD).

RESULTS OF THE ANALYSIS

The principal results of the analysis of post turbine fuel component conversion are shown in the attached spreadsheet tables (CAPSTN5.XLS) and Mathcad documents (CPSTONE5.MCD and CPSTONE6.MCD). The main results of the analyses are summarized as follows:

Catalytic Recuperator

- The $\Delta P/P$ calculations seem to very closely fit your measured values. [REDACTED] We chose as the best calculation of pressure drop an 800 cells/in² x 7-in. with 10% additional added length to describe the chevron geometry of the recuperator foils.
- The estimated averaged wall temperatures, or skin temperatures, within the recuperator seemed a little low ($< 50^{\circ}\text{F}$) based on [REDACTED] discussions of recuperator thermal efficiency. As a consequence, the cell size was increased to 600 cells/in² keeping the length the same (7 in. x 1.1) for a conservative calculation of mass transfer rates.
- For the mass transfer limited cases (assuming fast kinetics), virtually complete conversion CH_4 and CO is predicted (see Table of Results 1). Except at the highest power level, conversion of CH_4 and CO was essentially complete within the first inch or two of entry into the recuperator.
- For the transport-limited cases with C_7H_{14} , maximum conversions are low only for Case 5 (full power). Even in this case, 50 ppm would be converted to < 1 ppm (0.2 ppm) while concentrations entering the recuperator above 250 ppm would exit at levels above 1 ppm (500 ppm \Rightarrow 2.1 ppm). The situation improves for the other cases (e.g., Case 4 gives 500 ppm \Rightarrow 0.02 ppms while 5000 ppm \Rightarrow 0.17 ppm).
- Conversions would be much higher for transport limited conversion in a the 800 cells/in.² recuperator, as calculations with this cell size were found reproduce the observed pressure drop. In this case, the logarithm of the inlet concentration divided by the outlet concentration for all added components would be $\sim 35\%$ greater with the smaller cell size.
- The step-wise calculation which includes the temperature on flow velocity and transport properties showed reasonably good agreement with the integrated calculation using average properties. This method gave lower overall conversion than the averaged property formulas, but the results were close. Perhaps the higher property values at the inlet, particularly the greater velocity, more than offset the lower transport values at the outlet side.
- CH_4 conversion is catalytically rate limited under all conditions (see Table of Results 1). Conversions were calculated to be very low, with a maximum conversion of $\sim 66\%$ under Case 1 and $\sim 32\%$ conversion under Case 5. These conversions would increase somewhat, perhaps by a factor of 2, with the use of a thicker coating (e.g., 25 μm vs. 10 μm).
- CO conversion is likely to exceed 99% in all operating conditions for the recuperator. This is because the kinetics of CO conversion are probably much faster than CH_4 and may well be close to the transport-limited case, at least through the (hotter) first several inches of the recuperator where most of the CO would be consumed.

- The catalytic recuperator, C_7H_{14} rate determines its conversion in the recuperator conditions (see Table of Results 1). For the slower rates (derived from the rates for CH_4 oxidation) using the 600 cells/in.² value for recuperator cell size, we find a range from 99.4% conversion under Case 1 to about 85.6% under Case 5. If twice the rate of combustion of propane is extrapolated to the higher temperatures of the recuperator, much higher C_7H_{14} conversions result, 99.98% under Case 1, and 96.4% under Case 5.

Catalytic Monoliths

- The pressure drop reaches maximum specifications for the 400 cells/in.² honeycomb at 4-in. length. Maximum pressure drop would be reached in a shorter (~3.5 in. length) 600 cells/in.² monolith. Both configurations were chosen for analysis (CPSTONE5.MCD for 400 cells/in.² and CPSTONE6.MCD for 600 cells/in.²).
- Transport-limited conversion shows excellent performance for methane and CO in all cases, including the full-power case, for both honeycomb configurations (see Table of Results 2).
- As for the recuperator, methane conversion is again reaction rate limited (see Table of Results 3), with conversions range from 93.8% under Case 1 with the 600 cells/in.² monolith to only 31% conversion under Case 5 for the 400 cells/in.² monolith.
- C_7H_{14} conversions under transport-limited conditions depends on the specific configuration (see Table of Results 2). For the 600 cells/in.² monolith conversions are very high for Case 1, but fall to about 92% for Case 5. With the 400 cells/in.² configuration, these fast kinetic transport-limited conversions fall to 87% conversion under Case 5.
- The reaction rate of C_7H_{14} strongly affects its conversion in either honeycomb monolith (see Table of Results 3). For the extrapolated propane kinetics at 600 cells/in.², 98% conversion is expected under Case 5, whereas the 400 cells/in.² using the more conservative extrapolation using PdO methane kinetics, 86% conversion is expected under Case 5.

Effect of Washcoat Thermal Conductivity in a Recuperator

- The application of a thin washcoat of porous alumina gives a very slight increase in the overall heat transfer coefficient [REDACTED] (CPSNALT2.MCD). The thermal conductivity of the washcoat, while significantly less than that of stainless 321, is greater than that of the gas phase boundary. Because the washcoat displaces the gas phase (creating a narrower channel) it causes a slight increase in overall heat transfer coefficient.

OVERALL CONCLUSIONS AND RECOMMENDATIONS

The conclusions and recommendations drawn from the results of the analysis is listed below:

- 1) The actual C_7H_{14} outlet concentration from the turbine are needed to assess the effluent emissions in the high-power case (Case 5) for either control strategy. Provided that fast catalytic rates can be provided in washcoats on either the recuperator or upstream monoliths, maximum conversions for C_7H_{14} under full power range from 99.6% (for an effective cell size of 600 cells/in²) to > 99.9% (if the effective cell size is 800 cells/in²).
- 2) The two methods (averaged properties and integrated formulas vs. local temperature dependent properties and finite difference integration) show good agreement for recuperator performance with infinitely fast catalytic reactions at the wall.
- 3) Clearly, it will be necessary to apply and measure specific catalytic rates for C_7H_{14} or gasoline to be sure that these estimated conversions could be achieved under actual operating conditions for either the catalytic recuperator or the upstream honeycomb monoliths.
- 4) Thin wash coats (< 20 μ m) should have minimal effect on the transport of heat through the recuperator given the much greater resistance of the gas phase boundary layers.
- 5) For the current operating conditions, use of a standard 400 cells/in² x 4-in length catalytic monolith upstream of the recuperator is recommended.
- 6) If the recuperator temperature can be raised (~ 200°F) high conversions of CO, C_7H_{14} , and even CH_4 can be expected under all flow conditions. In this case it is possible that only the first 3 to 4 inches of the recuperator be wash coated with catalyst because the downstream wall temperatures are too cool to be effective.

Recupercator - Transport only (assumes fast reaction kinetics) at 600 cells/in2												
Inlet (added component) conc(ppm)	Case-1			Case-2			Case-3			Case-4		
	CH4	C7H14	CO	CH4	C7H14	CO	CH4	C7H14	CO	CH4	C7H14	CO
5000	2.011E-25	3.554E-05	5.555E-23	3.704E-19	0.002197	3.002E-17	1.373E-15	0.022664	5.542E-14	1.470E-12	0.1692	3.276E-11
2000	8.046E-26	1.422E-05	2.222E-23	1.481E-19	8.787E-04	1.201E-17	5.492E-16	0.03188	2.217E-14	5.880E-13	0.067483	1.310E-11
1000	4.023E-26	7.108E-06	1.111E-23	7.407E-20	4.393E-04	6.003E-18	2.746E-16	0.004593	1.108E-14	2.940E-12	0.033734	6.552E-11
500	2.011E-26	3.554E-06	5.555E-24	3.704E-20	2.197E-04	3.002E-18	1.373E-16	0.002298	5.542E-15	1.470E-13	0.016667	3.276E-12
200	8.046E-27	1.422E-06	2.222E-24	1.481E-20	8.787E-05	1.201E-18	5.492E-17	9.186E-04	2.217E-15	5.880E-14	0.0067468	1.310E-12
100	4.023E-27	7.108E-07	1.111E-24	7.407E-21	4.393E-05	6.003E-19	2.746E-17	4.593E-04	1.108E-15	2.940E-14	0.0033734	6.552E-13
50	2.011E-27	3.554E-07	5.555E-25	3.704E-21	2.197E-05	3.002E-19	1.373E-17	2.266E-04	5.542E-16	1.470E-14	0.0018887	3.276E-13
20	8.046E-28	1.422E-07	2.222E-25	1.481E-21	8.787E-06	1.201E-19	5.492E-18	9.186E-05	2.217E-16	5.880E-15	6.747E-04	1.310E-13
10	4.023E-28	7.108E-08	1.111E-25	7.407E-22	4.393E-06	6.003E-20	2.746E-18	4.593E-05	1.108E-16	2.940E-15	3.373E-04	6.552E-14
5	2.011E-28	3.554E-08	5.555E-26	3.704E-22	2.197E-06	3.002E-20	1.373E-18	2.266E-05	5.542E-17	1.470E-15	1.687E-04	3.276E-14
2	8.046E-29	1.422E-08	2.222E-26	1.481E-22	8.787E-07	1.201E-20	5.492E-19	9.186E-06	2.217E-17	5.880E-16	6.747E-05	1.310E-14
1	4.023E-29	7.108E-09	1.111E-26	7.407E-23	4.393E-07	6.003E-21	2.746E-19	4.593E-06	1.108E-17	2.940E-16	3.373E-05	6.552E-15

Recupercator - C7H14 without reaction with T-dependence (step) and CH4and C7H14 with finite catalytic reaction rates at the wall (C7H14 rate = 10 x CH4 Rate - slow kinetics)

Inlet conc(ppm)	Case-1			Case-2			Case-3			Case-4			Case-5		
	C7H14step	CH4react	C7H14react	C7H14step	CH4react	C7H14react	C7H14step	CH4react	C7H14react	C7H14step	CH4react	C7H14react	C7H14step	CH4react	C7H14react
5000	3.201E-04	1.675E-03	3.158E-03	0.012075	0.004830	0.004830	0.004830	0.004830	0.004830	0.004830	0.004830	0.004830	0.004830	0.004830	0.004830
2000	1.280E-04	6.70E-04	1.2634E-03	0.004830	0.004830	0.004830	0.004830	0.004830	0.004830	0.004830	0.004830	0.004830	0.004830	0.004830	0.004830
1000	6.402E-05	3.35E-04	6.317E-04	0.002415	0.002415	0.002415	0.002415	0.002415	0.002415	0.002415	0.002415	0.002415	0.002415	0.002415	0.002415
500	3.201E-05	1.675E-04	3.158E-04	0.001208	0.001208	0.001208	0.001208	0.001208	0.001208	0.001208	0.001208	0.001208	0.001208	0.001208	0.001208
200	1.280E-05	6.70E-05	1.2634E-04	0.000483	0.000483	0.000483	0.000483	0.000483	0.000483	0.000483	0.000483	0.000483	0.000483	0.000483	0.000483
100	6.402E-06	3.35E-05	6.317E-05	0.000242	0.000242	0.000242	0.000242	0.000242	0.000242	0.000242	0.000242	0.000242	0.000242	0.000242	0.000242
50	3.201E-06	1.675E-05	3.158E-05	0.000121	0.000121	0.000121	0.000121	0.000121	0.000121	0.000121	0.000121	0.000121	0.000121	0.000121	0.000121
20	1.280E-06	6.70E-06	1.2634E-05	0.000048	0.000048	0.000048	0.000048	0.000048	0.000048	0.000048	0.000048	0.000048	0.000048	0.000048	0.000048
10	6.402E-07	3.35E-06	6.317E-06	0.000024	0.000024	0.000024	0.000024	0.000024	0.000024	0.000024	0.000024	0.000024	0.000024	0.000024	0.000024
5	3.201E-07	1.675E-06	3.158E-06	0.000012	0.000012	0.000012	0.000012	0.000012	0.000012	0.000012	0.000012	0.000012	0.000012	0.000012	0.000012
2	1.280E-07	6.70E-07	1.2634E-06	0.000004	0.000004	0.000004	0.000004	0.000004	0.000004	0.000004	0.000004	0.000004	0.000004	0.000004	0.000004
1	6.402E-08	3.35E-07	6.317E-07	0.000002	0.000002	0.000002	0.000002	0.000002	0.000002	0.000002	0.000002	0.000002	0.000002	0.000002	0.000002

Case1: 1 2 3 4 5
In(yout)/ln

CH4:	-65.383	-50.957	-42.739	-35.763	-18.994
C7H14	-18.762	-14.638	-12.291	-10.297	-5.49
CO	-59.762	-46.562	-39.041	-32.659	-17.344
C7H14step	-16.56407	-12.933811	-10.88112	-9.142682	-4.968427
CH4react	-1.0936247	-0.8843077	-0.77219	-0.675307	-0.379797
C7H14react	-5.0645109	-4.0989552	-3.581641	-3.133396	-1.955456

BL transport only with averaged integrated values
BL transport only with averaged integrated values
BL transport only with averaged integrated values
BL transport only with T-dependent properties and step-wise integration
BL transport-restricted catalytic rates with T-dependent properties and step-wise integration
BL transport-restricted catalytic rates with T-dependent properties and step-wise integration

Table of Results 2

Transport only (assumes fast reaction kinetics) for a 600 cells/in ² x 3.5-in length square honeycomb monolith																
Inlet (added component)	Case-1		Case-2		Case-3		Case-4		Case-5							
	CH4	C7H14	CO	CH4	C7H14	CO	CH4	C7H14	CO	CH4	C7H14	CO	CH4	C7H14	CO	
5000	7.960E-25	4.179E-04	2.470E-22	2.089E-18	0.017828	1.708E-16	9.839E-15	0.1545	3.802E-13	1.170E-11	0.8353	2.395E-10	2.773E-04	0.003858	0.001222	
2000	3.184E-25	1.672E-04	9.878E-23	8.276E-19	0.007111	6.831E-17	3.939E-15	0.081818	1.521E-13	4.878E-12	0.3743	9.582E-11	1.109E-04	0.013544	4.890E-04	
1000	1.592E-25	8.359E-05	4.939E-23	4.138E-18	0.003586	3.415E-17	1.989E-15	0.030803	7.604E-14	2.339E-12	0.1871	4.781E-11	5.546E-05	0.019722	2.445E-04	
500	7.960E-26	4.179E-05	2.470E-23	2.089E-19	0.001793	1.708E-17	9.839E-16	0.015452	3.802E-14	1.170E-12	0.083528	2.395E-11	2.773E-05	0.013388	1.222E-04	
200	3.184E-26	1.672E-05	9.878E-24	8.276E-20	0.000717	6.831E-18	3.939E-16	0.008181	1.521E-14	4.878E-13	0.037433	9.582E-12	1.109E-05	0.013154	4.890E-05	
100	1.592E-26	8.359E-06	4.939E-24	4.138E-20	0.000359	3.415E-18	1.989E-16	0.003090	7.604E-15	2.339E-13	0.018708	4.791E-12	5.546E-06	0.014072	2.445E-05	
50	7.960E-27	4.179E-06	2.470E-24	2.089E-20	0.000179	1.708E-18	9.839E-17	0.001545	3.802E-15	1.170E-13	0.008353	2.395E-12	2.773E-06	0.017039	1.222E-05	
20	3.184E-27	1.672E-06	9.878E-25	8.276E-21	7.171E-05	6.831E-19	3.939E-17	6.181E-04	1.521E-15	4.878E-14	0.003743	9.582E-13	1.109E-06	0.02815	4.890E-06	
10	1.592E-27	8.359E-07	4.939E-25	4.138E-21	3.586E-05	3.415E-19	1.989E-17	3.090E-04	7.604E-16	2.339E-14	0.001871	4.791E-13	5.546E-07	0.01408	2.445E-06	
5	7.960E-28	4.179E-07	2.470E-25	2.089E-21	1.783E-05	1.708E-19	9.839E-18	1.545E-04	3.802E-16	1.170E-14	9.353E-04	2.395E-13	2.773E-07	0.010386	1.222E-06	
2	3.184E-28	1.672E-07	9.878E-26	8.276E-22	7.171E-06	6.831E-20	3.939E-18	6.181E-05	1.521E-16	4.878E-15	3.741E-04	9.582E-14	1.109E-07	0.028154	4.890E-07	
1	1.592E-28	8.359E-08	4.939E-26	4.138E-22	3.586E-06	3.415E-20	1.989E-18	3.090E-05	7.604E-17	2.339E-15	1.871E-04	4.791E-14	5.546E-08	0.014072	2.445E-07	
Transport only (assumes fast reaction kinetics) for a 400 cells/in ² x 4-in length square honeycomb monolith																
Inlet concn(ppm)	Case-1		Case-2		Case-3		Case-4		Case-5							
	CH4	C7H14	CO	CH4	C7H14	CO	CH4	C7H14	CO	CH4	C7H14	CO	CH4	C7H14	CO	
5000	3.307E-18	0.003426	2.617E-16	2.551E-13	0.090292	7.363E-12	1.816E-10	0.5992	2.615E-09	3.558E-08	2.81585934	3.550E-07	0.01476631	0.013333	0.045698	
2000	1.323E-18	0.001370	1.047E-16	1.021E-13	0.036117	2.945E-12	6.463E-11	0.2353	1.046E-09	1.423E-08	1.12628608	1.420E-07	0.00590853	0.018279	0.018279	
1000	6.613E-19	6.852E-04	5.234E-17	5.103E-14	0.018058	1.473E-12	3.231E-11	0.1178	5.230E-10	7.115E-09	0.56313003	7.100E-08	0.00288328	0.008779	0.008140	
500	3.307E-19	3.426E-04	2.617E-17	2.551E-14	0.008028	7.363E-13	1.616E-11	0.059825	2.615E-10	3.558E-09	0.28156501	3.550E-08	0.00147683	0.004570	0.004570	
200	1.323E-19	1.370E-04	1.047E-17	1.021E-14	0.003512	2.945E-13	6.463E-12	0.023330	1.046E-10	1.423E-09	0.11262801	1.420E-08	5.907E-04	0.001828	0.001828	
100	6.613E-20	6.852E-05	5.234E-18	5.103E-15	0.01806	1.473E-13	3.231E-12	0.014785	5.230E-11	7.115E-10	0.056313	7.100E-09	2.853E-04	0.002878	9.140E-04	
50	3.307E-20	3.426E-05	2.617E-18	2.551E-15	9.029E-04	7.363E-14	1.616E-12	0.005882	2.615E-11	3.558E-10	0.0012628	3.550E-09	1.477E-04	0.001839	4.570E-04	
20	1.323E-20	1.370E-05	1.047E-18	1.021E-15	3.612E-04	2.945E-14	6.463E-13	0.002353	1.046E-11	1.423E-10	0.0012628	3.550E-09	5.907E-05	0.001839	4.570E-04	
10	6.613E-21	6.852E-06	5.234E-19	5.103E-16	1.806E-04	1.473E-14	3.231E-13	0.001178	5.230E-12	7.115E-11	0.0056313	7.100E-10	2.935E-05	0.02388	9.140E-04	
5	3.307E-21	3.426E-06	2.617E-19	2.551E-16	9.029E-05	7.363E-15	1.616E-13	5.882E-04	2.615E-12	3.558E-11	0.00281565	3.550E-10	1.477E-05	0.01184	4.570E-05	
2	1.323E-21	1.370E-06	1.047E-19	1.021E-16	3.612E-05	2.945E-15	6.463E-14	2.353E-04	1.046E-12	1.423E-11	0.00112628	1.420E-10	5.907E-06	0.004756	1.828E-05	
1	6.613E-22	6.852E-07	5.234E-20	5.103E-17	1.806E-05	1.473E-15	3.231E-14	1.178E-04	5.230E-13	7.115E-12	5.831E-04	7.100E-11	2.953E-06	0.0028878	9.140E-06	
Case#:																
	1	2	3	4	5											
CH4-600	-64.0074	-49.2367	-40.7696	-33.689	-16.7078	BL transport only with averaged intergrated values										
CH7H4-600	-16.2974	-12.5386	-10.3846	-8.5841	-4.2632	BL transport only with averaged intergrated values										
CO-600	-58.27	-44.8234	-37.1153	-30.6695	-15.2241	BL transport only with averaged intergrated values										
CH4-400	-48.7678	-37.5142	-31.0633	-25.6888	-12.7326	BL transport only with averaged intergrated values										
C7H14-400	-14.1935	-10.9218	-9.0478	-7.482	-3.7348	BL transport only with averaged intergrated values										
CO-400	-44.3968	-34.1518	-28.2792	-23.3684	-11.6029	BL transport only with averaged intergrated values										

Inlet (added component)	C7H14 with finite catalytic reaction rates at the wall (slow C7H14 rate = 10 x CH4 rate; moderate C7H14 rate = 2 x C3H8 rate)																									
	Case-1					Case-2					Case-3					Case-4					Case-5					
conc(ppm)	Recup-m	400cpl-s	Recup-m	600cpl-m	400cpl-s	Recup-m	600cpl-m	400cpl-s	Recup-m	600cpl-m	400cpl-s	Recup-m	600cpl-m	400cpl-s	Recup-m	600cpl-m	400cpl-s	Recup-m	600cpl-m	400cpl-s	Recup-m	600cpl-m	400cpl-s	Recup-m	600cpl-m	400cpl-s
5000	1.1680	0.001005	0.7803	0.035610	0.11598	0.7109	0.035610	0.11598	0.7109	0.035610	0.11598	0.7109	0.035610	0.11598	0.7109	0.035610	0.11598	0.7109	0.035610	0.11598	0.7109	0.035610	0.11598	0.7109	0.035610	0.11598
2000	0.4672	4.020E-04	0.7162	0.014244	4.4866	0.3400	0.014244	4.4866	0.3400	0.014244	4.4866	0.3400	0.014244	4.4866	0.3400	0.014244	4.4866	0.3400	0.014244	4.4866	0.3400	0.014244	4.4866	0.3400	0.014244	4.4866
1000	0.2336	2.010E-04	0.3881	0.007122	2.2306	0.1700	0.007122	2.2306	0.1700	0.007122	2.2306	0.1700	0.007122	2.2306	0.1700	0.007122	2.2306	0.1700	0.007122	2.2306	0.1700	0.007122	2.2306	0.1700	0.007122	2.2306
500	0.1168	1.005E-04	0.1941	0.003561	1.1150	0.8710	0.003561	1.1150	0.8710	0.003561	1.1150	0.8710	0.003561	1.1150	0.8710	0.003561	1.1150	0.8710	0.003561	1.1150	0.8710	0.003561	1.1150	0.8710	0.003561	1.1150
200	0.04672	4.020E-05	0.07803	0.001424	0.4460	0.3400	0.001424	0.4460	0.3400	0.001424	0.4460	0.3400	0.001424	0.4460	0.3400	0.001424	0.4460	0.3400	0.001424	0.4460	0.3400	0.001424	0.4460	0.3400	0.001424	0.4460
100	0.02336	2.010E-05	0.03881	0.000712	0.2231	0.1700	0.000712	0.2231	0.1700	0.000712	0.2231	0.1700	0.000712	0.2231	0.1700	0.000712	0.2231	0.1700	0.000712	0.2231	0.1700	0.000712	0.2231	0.1700	0.000712	0.2231
50	0.01168	1.005E-05	0.01941	0.000356	0.1115	0.8710	0.000356	0.1115	0.8710	0.000356	0.1115	0.8710	0.000356	0.1115	0.8710	0.000356	0.1115	0.8710	0.000356	0.1115	0.8710	0.000356	0.1115	0.8710	0.000356	0.1115
20	0.004672	4.020E-06	0.007803	0.000142	0.1244	0.3400	0.000142	0.1244	0.3400	0.000142	0.1244	0.3400	0.000142	0.1244	0.3400	0.000142	0.1244	0.3400	0.000142	0.1244	0.3400	0.000142	0.1244	0.3400	0.000142	0.1244
10	0.002336	2.010E-06	0.003881	0.000071	0.1142	0.1700	0.000071	0.1142	0.1700	0.000071	0.1142	0.1700	0.000071	0.1142	0.1700	0.000071	0.1142	0.1700	0.000071	0.1142	0.1700	0.000071	0.1142	0.1700	0.000071	0.1142
5	0.001168	1.005E-06	0.001941	0.000036	0.0557	0.0871	0.000036	0.0557	0.0871	0.000036	0.0557	0.0871	0.000036	0.0557	0.0871	0.000036	0.0557	0.0871	0.000036	0.0557	0.0871	0.000036	0.0557	0.0871	0.000036	0.0557
2	0.000584	5.025E-07	0.000970	0.000018	0.0278	0.0435	0.000018	0.0278	0.0435	0.000018	0.0278	0.0435	0.000018	0.0278	0.0435	0.000018	0.0278	0.0435	0.000018	0.0278	0.0435	0.000018	0.0278	0.0435	0.000018	0.0278
1	0.000292	2.512E-07	0.000485	0.000009	0.0139	0.0218	0.000009	0.0139	0.0218	0.000009	0.0139	0.0218	0.000009	0.0139	0.0218	0.000009	0.0139	0.0218	0.000009	0.0139	0.0218	0.000009	0.0139	0.0218	0.000009	0.0139
C7H14 without reaction and CH4 with finite catalytic reaction rates at the wall																										
Inlet conc(ppm)	Case-1					Case-2					Case-3					Case-4					Case-5					
	C7H14	CH4H800	CH4H400	C7H14	CH4H800	C7H14	CH4H800	CH4H400	C7H14	CH4H800	C7H14	CH4H800	CH4H400	C7H14	CH4H800	C7H14	CH4H800	CH4H400	C7H14	CH4H800	C7H14	CH4H800	CH4H400	C7H14	CH4H800	CH4H400
5000	3.201E-04	3.1000	3.6130	0.012075	0.012075	0.012075	0.012075	0.012075	0.012075	0.012075	0.012075	0.012075	0.012075	0.012075	0.012075	0.012075	0.012075	0.012075	0.012075	0.012075	0.012075	0.012075	0.012075	0.012075	0.012075	
2000	1.280E-04	1.2400	1.5652	0.004830	0.004830	0.004830	0.004830	0.004830	0.004830	0.004830	0.004830	0.004830	0.004830	0.004830	0.004830	0.004830	0.004830	0.004830	0.004830	0.004830	0.004830	0.004830	0.004830	0.004830	0.004830	
1000	6.402E-05	6.2000	7.8260	0.002415	0.002415	0.002415	0.002415	0.002415	0.002415	0.002415	0.002415	0.002415	0.002415	0.002415	0.002415	0.002415	0.002415	0.002415	0.002415	0.002415	0.002415	0.002415	0.002415	0.002415	0.002415	
500	3.201E-05	3.1000	3.9130	0.001208	0.001208	0.001208	0.001208	0.001208	0.001208	0.001208	0.001208	0.001208	0.001208	0.001208	0.001208	0.001208	0.001208	0.001208	0.001208	0.001208	0.001208	0.001208	0.001208	0.001208	0.001208	
200	1.280E-05	1.2400	1.5652	0.000604	0.000604	0.000604	0.000604	0.000604	0.000604	0.000604	0.000604	0.000604	0.000604	0.000604	0.000604	0.000604	0.000604	0.000604	0.000604	0.000604	0.000604	0.000604	0.000604	0.000604	0.000604	
100	6.402E-06	6.2000	7.8260	0.000302	0.000302	0.000302	0.000302	0.000302	0.000302	0.000302	0.000302	0.000302	0.000302	0.000302	0.000302	0.000302	0.000302	0.000302	0.000302	0.000302	0.000302	0.000302	0.000302	0.000302	0.000302	
50	3.201E-06	3.1000	3.9130	0.000151	0.000151	0.000151	0.000151	0.000151	0.000151	0.000151	0.000151	0.000151	0.000151	0.000151	0.000151	0.000151	0.000151	0.000151	0.000151	0.000151	0.000151	0.000151	0.000151	0.000151	0.000151	
20	1.280E-06	1.2400	1.5652	0.000075	0.000075	0.000075	0.000075	0.000075	0.000075	0.000075	0.000075	0.000075	0.000075	0.000075	0.000075	0.000075	0.000075	0.000075	0.000075	0.000075	0.000075	0.000075	0.000075	0.000075	0.000075	
10	6.402E-07	6.2000	7.8260	0.000038	0.000038	0.000038	0.000038	0.000038	0.000038	0.000038	0.000038	0.000038	0.000038	0.000038	0.000038	0.000038	0.000038	0.000038	0.000038	0.000038	0.000038	0.000038	0.000038	0.000038	0.000038	
5	3.201E-07	3.1000	3.9130	0.000019	0.000019	0.000019	0.000019	0.000019	0.000019	0.000019	0.000019	0.000019	0.000019	0.000019	0.000019	0.000019	0.000019	0.000019	0.000019	0.000019	0.000019	0.000019	0.000019	0.000019	0.000019	
2	1.280E-07	1.2400	1.5652	0.000009	0.000009	0.000009	0.000009	0.000009	0.000009	0.000009	0.000009	0.000009	0.000009	0.000009	0.000009	0.000009	0.000009	0.000009	0.000009	0.000009	0.000009	0.000009	0.000009	0.000009	0.000009	
1	6.402E-08	6.2000	7.8260	0.000005	0.000005	0.000005	0.000005	0.000005	0.000005	0.000005	0.000005	0.000005	0.000005	0.000005	0.000005	0.000005	0.000005	0.000005	0.000005	0.000005	0.000005	0.000005	0.000005	0.000005	0.000005	
In(yout)/in																										
Case#	1	2	3	4	5																					
C7H14Rs	2.34E-04	1.14E-03	2.67E-03	5.56E-03	3.60E-02																					
C7H14H800s	2.01E-07	7.12E-08	5.43E-05	2.99E-03	1.99E-02																					
C7H14H400s	3.58E-04	2.23E-03	6.34E-03	1.52E-02	1.46E-01																					
C7H14R	-16.56407	-12.933611	-10.881122	-9.1426817	-4.966427																					
CH4H800	0.062	0.118	0.1705	0.232	0.5693																					
CH4H400	0.07826	0.1411	0.1977	0.2621	0.5959																					

BL transport-restricted slower catalytic rates with T-dependent properties and step-wise integration
 BL transport-restricted moderate catalytic rates with T-dependent properties and step-wise integration
 BL transport-restricted slower catalytic rates with T-dependent properties and step-wise integration
 BL transport only with T-dependent properties and step-wise integration
 BL transport-restricted catalytic rates with T-dependent properties and step-wise integration
 BL transport-restricted catalytic rates with T-dependent properties and step-wise integration

 Gas Properties and Constants

$$\begin{aligned} \text{cm} &= 0.01 \cdot \text{m} & \text{J} &= \text{kg} \cdot \text{m}^2 \cdot \text{sec}^{-2} & \text{W} &= \text{J} \cdot \text{sec}^{-1} & \text{Pref} &= 1 \cdot \text{atm} \\ \text{N} &= \text{kg} \cdot \text{m} \cdot \text{sec}^{-2} & \text{Pa} &= \text{N} \cdot \text{m}^{-2} & \text{atm} &= 101300 \cdot \text{Pa} & \mu\text{m} &= 0.000001 \cdot \text{m} \\ R &= 8.3143 \cdot \frac{\text{J}}{\text{K}} & R_c &= 8.3143 \cdot \text{J} \cdot \text{mole}^{-1} \cdot \text{K}^{-1} \end{aligned}$$

n	Gas	MolWt	$\sigma(\text{LJ})$	$\epsilon(\text{LJ})$
0	CH4	MW ₀ = 16.044·gm	$\sigma_0 = 3.785 \cdot 10^{-10} \cdot \text{m}$	$\epsilon_0 = 148.6 \cdot \text{K}$
1	O2	MW ₁ = 31.999·gm	$\sigma_1 = 3.464 \cdot 10^{-10} \cdot \text{m}$	$\epsilon_1 = 106.7 \cdot \text{K}$
2	N2	MW ₂ = 28.018·gm	$\sigma_2 = 3.798 \cdot 10^{-10} \cdot \text{m}$	$\epsilon_2 = 71.4 \cdot \text{K}$
3	CO2	MW ₃ = 44.010·gm	$\sigma_3 = 3.941 \cdot 10^{-10} \cdot \text{m}$	$\epsilon_3 = 195.2 \cdot \text{K}$
4	H2O	MW ₄ = 18.015·gm	$\sigma_4 = 2.641 \cdot 10^{-10} \cdot \text{m}$	$\epsilon_4 = 809.1 \cdot \text{K}$
5	C7H14 methyl-cyclohexane		Tc7 = 572.2·K Tb7 = 374.1·K Pc7 = 3.47·10 ⁶ ·Pa Vc7 = 368	
			$\epsilon_5 = \frac{Tc7}{1.2593}$	$\sigma_5 = Vc7^{\frac{1}{3}} \cdot 10^{-10} \cdot \text{m}$
		MW ₅ = 98.189·gm	$\sigma_5 = 7.1661 \cdot 10^{-10} \cdot \text{m}$	$\epsilon_5 = 454.3794 \cdot \text{K}$
6	CO	MW ₆ = 28.01·gm	$\sigma_6 = 3.69 \cdot 10^{-10} \cdot \text{m}$	$\epsilon_6 = 91.7 \cdot \text{K}$

 Define constants for transport integrals:

$$\begin{aligned} \sigma\mu a_0 &= 1.16145 & \sigma\mu b_0 &= 0.14874 & \sigma Da_0 &= 1.06036 & \sigma Db_0 &= 0.1561 \\ \sigma\mu a_1 &= 0.52487 & \sigma\mu b_1 &= 0.7732 & \sigma Da_1 &= 0.193 & \sigma Db_1 &= 0.47635 \\ \sigma\mu a_2 &= 2.16178 & \sigma\mu b_2 &= 2.43787 & \sigma Da_2 &= 1.03587 & \sigma Db_2 &= 1.52996 \\ & & & & \sigma Da_3 &= 1.76474 & \sigma Db_3 &= 3.89411 \end{aligned}$$

Define transport integrals:

$$\begin{aligned} \Omega\mu(T) &= \sigma\mu a_0 \cdot \exp(-\sigma\mu b_0 \cdot \ln(T)) + \sum_{i\mu=1}^2 \sigma\mu a_{i\mu} \cdot \exp(-\sigma\mu b_{i\mu} \cdot T) & \Omega\mu(3) &= 1.0394 \\ \Omega D(T) &= \sigma Da_0 \cdot \exp(-\sigma Db_0 \cdot \ln(T)) + \sum_{i\mu=1}^3 \sigma Da_{i\mu} \cdot \exp(-\sigma Db_{i\mu} \cdot T) & \Omega D(3) &= 0.95002 \end{aligned}$$

Set Inlet Conditions:

$$P = 1 \text{ atm}$$

$$\phi = 0.1$$

$$y_{adc7} = 0.0021859$$

This value for y_{adc7} was determined via enthalpy functions [REDACTED] for temperature rise from 1000F to 1511F.

$$y_{eqc7} = \phi \cdot \frac{0.205}{14}$$

$$\phi_{eq} = \phi \cdot \frac{y_{adc7}}{y_{eqc7}}$$

$$y_{eqc7} = 0.001464$$

$$\phi_{eq} = 0.149281$$

The value for y_{eq} was determined for a given equivalence ratio of 0.1 in moist air

Define gas composition with C7H14 fuel using moist (2%) air:

09933663-082201

$$y_7(y_0, x) = \frac{\begin{bmatrix} 0 \\ (1 - y_0) \cdot 0.205 - 10.5 \cdot y_0 \cdot x \\ (1 - y_0) \cdot 0.775 \\ 7 \cdot (y_0 \cdot x) \\ (1 - y_0) \cdot 0.02 + 7 \cdot y_0 \cdot x \\ y_0 \cdot (1 - x) \\ 0 \end{bmatrix}}{1 + 2.5 \cdot y_0 \cdot x}$$

$$y_{eq} := y_7(y_{eqc7}, 1)$$

$$y_{ad} := y_7(y_{adc7}, 1)$$

$$y_{eq} = \begin{bmatrix} 0 \\ 0.188634 \\ 0.771043 \\ 0.010213 \\ 0.03011 \\ 0 \\ 0 \end{bmatrix}$$

$$y_{ad} = \begin{bmatrix} 0 \\ 0.180613 \\ 0.769103 \\ 0.015218 \\ 0.035066 \\ 0 \\ 0 \end{bmatrix}$$

Define functions for evaluation of mixture properties (ideal gas) for complete fuel conversion and a given temperature.

Density and average molecular weight:

$$\rho_{mix}(T) = \left(\sum_{kk=0}^6 y_{eq_{kk}} \cdot MW_{kk} \right) \cdot \frac{P}{R \cdot T}$$

$$MW_{mix} = \left(\sum_{kk=0}^6 y_{eq_{kk}} \cdot MW_{kk} \right)$$

$$\rho_{mix}(300 \cdot K) = 1.162787 \cdot \text{kg} \cdot \text{m}^{-3}$$

$$MW_{mix} = 28.631 \cdot \text{gm}$$

Define diffusion coefficients for specific binary diffusion pairs:

$$\text{Diff}(n, m, T) = 1.8829 \cdot 10^{-27} \cdot \left[\left(\frac{1}{\text{MW}_n} + \frac{1}{\text{MW}_m} \right) \cdot T^3 \right]^{0.5} \cdot 10^8 \cdot \text{gm}^{0.5} \cdot \text{cm}^4 \cdot \text{sec}^{-1} \cdot \text{K}^{-1.5} \cdot \left(\frac{\sigma_n + \sigma_m}{2} \right)^2 \cdot \Omega_D \left[\frac{T}{(\epsilon_n \cdot \epsilon_m)^{0.5}} \right] \cdot \frac{P}{\text{Pref}}$$

$$\text{Diff}(0, 2, 300 \cdot \text{K}) = 0.2225 \cdot \text{sec}^{-1} \cdot \text{cm}^2$$

$$\text{Diff}(2, 6, 300 \cdot \text{K}) = 0.207 \cdot \text{sec}^{-1} \cdot \text{cm}^2$$

Define functions for use with various fuel-air mixtures:

$$\text{Dch4}(T) = \frac{1}{\sum_{j\text{gas}=1}^4 \frac{\text{yeq}_{j\text{gas}}}{\text{Diff}(0, j\text{gas}, T)}}$$

$$\text{Dch4}(298 \cdot \text{K}) = 2.1912 \cdot 10^{-5} \cdot \text{m}^2 \cdot \text{sec}^{-1}$$

$$\text{Dc7h14}(T) = \frac{1}{\sum_{j\text{gas}=1}^4 \frac{\text{yeq}_{j\text{gas}}}{\text{Diff}(5, j\text{gas}, T)}}$$

$$\text{Dc7h14}(298 \cdot \text{K}) = 5.8372 \cdot 10^{-6} \cdot \text{m}^2 \cdot \text{sec}^{-1}$$

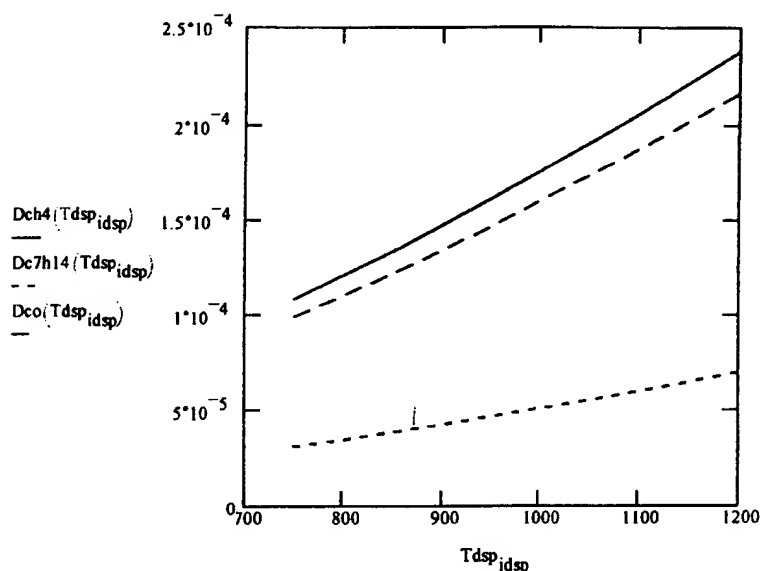
$$\text{Dco}(T) = \frac{1}{\sum_{j\text{gas}=1}^4 \frac{\text{yeq}_{j\text{gas}}}{\text{Diff}(6, j\text{gas}, T)}}$$

$$\text{Dco}(298 \cdot \text{K}) = 2.0451 \cdot 10^{-5} \cdot \text{m}^2 \cdot \text{sec}^{-1}$$

Display gas mixture properties

$$\text{idsp} = 0..9 \quad \text{Tin} := \left[(1000 - 32) \cdot \frac{5}{9} + 273.15 \right] \cdot \text{K} \quad \text{Tin} = 810.9278 \cdot \text{K}$$

$$\text{Tdsp}_{\text{idsp}} = (750 + 50 \cdot \text{idsp}) \cdot \text{K} \quad \text{Tout} := \left[(1511 - 32) \cdot \frac{5}{9} + 273.15 \right] \cdot \text{K} \quad \text{Tout} = 1094.8167 \cdot \text{K}$$



0993363"033701

T_{dsp_idsp}	$D_{ch4}(T_{dsp_idsp})$	$D_{c7h14}(T_{dsp_idsp})$	$D_{co}(T_{dsp_idsp})$
$7.5 \cdot 10^2 \cdot K$	$1.082 \cdot 10^{-4} \cdot m^2 \cdot sec^{-1}$	$3.1097 \cdot 10^{-5} \cdot m^2 \cdot sec^{-1}$	$9.8836 \cdot 10^{-5} \cdot m^2 \cdot sec^{-1}$
$8 \cdot 10^2 \cdot K$	$1.2064 \cdot 10^{-4} \cdot m^2 \cdot sec^{-1}$	$3.4776 \cdot 10^{-5} \cdot m^2 \cdot sec^{-1}$	$1.101 \cdot 10^{-4} \cdot m^2 \cdot sec^{-1}$
$8.5 \cdot 10^2 \cdot K$	$1.3359 \cdot 10^{-4} \cdot m^2 \cdot sec^{-1}$	$3.8613 \cdot 10^{-5} \cdot m^2 \cdot sec^{-1}$	$1.2184 \cdot 10^{-4} \cdot m^2 \cdot sec^{-1}$
$9 \cdot 10^2 \cdot K$	$1.4705 \cdot 10^{-4} \cdot m^2 \cdot sec^{-1}$	$4.2603 \cdot 10^{-5} \cdot m^2 \cdot sec^{-1}$	$1.3402 \cdot 10^{-4} \cdot m^2 \cdot sec^{-1}$
$9.5 \cdot 10^2 \cdot K$	$1.61 \cdot 10^{-4} \cdot m^2 \cdot sec^{-1}$	$4.6743 \cdot 10^{-5} \cdot m^2 \cdot sec^{-1}$	$1.4665 \cdot 10^{-4} \cdot m^2 \cdot sec^{-1}$
$1 \cdot 10^3 \cdot K$	$1.7543 \cdot 10^{-4} \cdot m^2 \cdot sec^{-1}$	$5.1031 \cdot 10^{-5} \cdot m^2 \cdot sec^{-1}$	$1.5972 \cdot 10^{-4} \cdot m^2 \cdot sec^{-1}$
$1.05 \cdot 10^3 \cdot K$	$1.9033 \cdot 10^{-4} \cdot m^2 \cdot sec^{-1}$	$5.5462 \cdot 10^{-5} \cdot m^2 \cdot sec^{-1}$	$1.7322 \cdot 10^{-4} \cdot m^2 \cdot sec^{-1}$
$1.1 \cdot 10^3 \cdot K$	$2.057 \cdot 10^{-4} \cdot m^2 \cdot sec^{-1}$	$6.0035 \cdot 10^{-5} \cdot m^2 \cdot sec^{-1}$	$1.8714 \cdot 10^{-4} \cdot m^2 \cdot sec^{-1}$
$1.15 \cdot 10^3 \cdot K$	$2.2152 \cdot 10^{-4} \cdot m^2 \cdot sec^{-1}$	$6.4746 \cdot 10^{-5} \cdot m^2 \cdot sec^{-1}$	$2.0148 \cdot 10^{-4} \cdot m^2 \cdot sec^{-1}$
$1.2 \cdot 10^3 \cdot K$	$2.378 \cdot 10^{-4} \cdot m^2 \cdot sec^{-1}$	$6.9593 \cdot 10^{-5} \cdot m^2 \cdot sec^{-1}$	$2.1624 \cdot 10^{-4} \cdot m^2 \cdot sec^{-1}$

Define interpolation formulas for D_{ch4} , D_{c7h14} , and D_{co} vs. $T(K)$ via Jandel Scientific's Tablecurve program

$$D_{ch4T}(T) = \exp\left(-10.623294 + 1.6259688 \cdot \ln\left(\frac{T}{K}\right) - \frac{46.41736 \cdot K}{T}\right) \cdot \frac{cm^2}{sec}$$

$$D_{ch4}(1000 \cdot K) = 1.75426 \cdot sec^{-1} \cdot cm^2$$

$$D_{ch4T}(1000 \cdot K) = 1.75432 \cdot sec^{-1} \cdot cm^2$$

$$D_{c7h14T}(T) = \exp\left(11.822189 + 1.6260138 \cdot \ln\left(\frac{T}{K}\right) - \frac{82.65375 \cdot K}{T}\right) \cdot \frac{cm^2}{sec}$$

$$D_{c7h14}(1000 \cdot K) = 0.51031 \cdot sec^{-1} \cdot cm^2$$

$$D_{c7h14T}(1000 \cdot K) = 0.51031 \cdot sec^{-1} \cdot cm^2$$

$$D_{coT}(T) = \exp\left(10.831955 + 1.6394196 \cdot \ln\left(\frac{T}{K}\right) - 24.53899 \cdot \frac{K}{T}\right) \cdot cm^2 \cdot sec^{-1}$$

$$D_{co}(1000 \cdot K) = 1.59722 \cdot sec^{-1} \cdot cm^2$$

$$D_{coT}(1000 \cdot K) = 1.59714 \cdot sec^{-1} \cdot cm^2$$

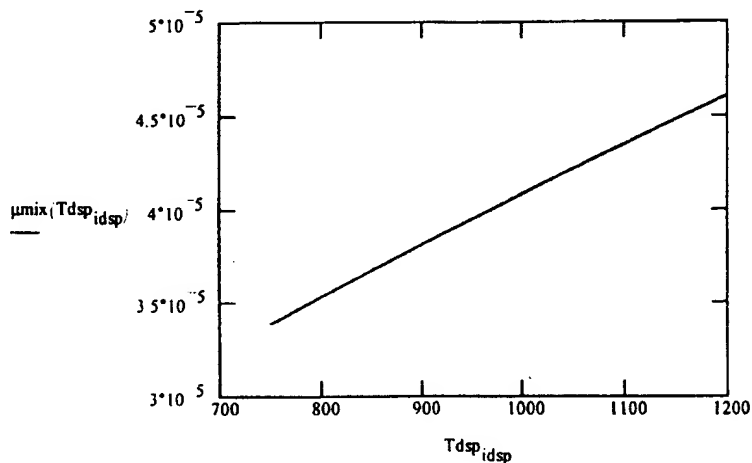
Define viscosity functions for major constituents:

$$\mu(T) := \frac{2.6693 \cdot 10^{-26} \cdot \left(\frac{MW_0 \cdot T}{(\sigma_0)^2 \cdot \Omega \mu \left(\frac{T}{\epsilon_0} \right)} \right)^{0.5} \cdot \frac{10^5 \cdot \text{cm}}{\text{sec}} \cdot \left(\frac{\text{gm}}{\text{K}} \right)^{0.5}}{\frac{1.116 \cdot (MW_4 \cdot T)^{0.5}}{(3.115 \cdot 10^{-8} \cdot \text{cm})^2 \cdot \Omega \mu \left(\frac{T}{514 \cdot \text{K}} \right)} \cdot \left[2.6693 \cdot 10^{-26} \cdot \left(\frac{10^5 \cdot \text{cm}}{\text{sec}} \right) \cdot \left(\frac{\text{gm}}{\text{K}} \right)^{0.5} \right]}$$

$$\mu(300 \cdot \text{K}) = \begin{bmatrix} 1.10281 \cdot 10^{-5} \\ 2.0603 \cdot 10^{-5} \\ 1.76981 \cdot 10^{-5} \\ 1.51851 \cdot 10^{-5} \\ 1.06784 \cdot 10^{-5} \end{bmatrix} \cdot \text{kg} \cdot \text{m}^{-1} \cdot \text{sec}^{-1}$$

$$\mu_{\text{mix}}(T) := \sum_{n=1}^4 \frac{y_{eq_n} \cdot \mu(T)_n}{\sum_{m=1}^4 y_{eq_m} \cdot \frac{\left[1 + \left(\frac{\mu(T)_n}{\mu(T)_m} \right)^{0.5} \cdot \left(\frac{MW_m}{MW_n} \right)^{0.25} \right]^2}{\left[8 \cdot \left(1 + \frac{MW_n}{MW_m} \right) \right]^{0.5}}}}$$

$$y_{eq} = \begin{bmatrix} 0 \\ 0.1886 \\ 0.771 \\ 0.0102 \\ 0.0301 \\ 0 \\ 0 \end{bmatrix}$$



Tdsp_idsp

750-K
800-K
850-K
900-K
950-K
1000-K
1050-K
1100-K
1150-K
1200-K

 $\mu_{\text{mix}}(T_{\text{dsp_idsp}})$

$3.3875 \cdot 10^{-5} \cdot \text{kg} \cdot \text{m}^{-1} \cdot \text{sec}^{-1}$
$3.5348 \cdot 10^{-5} \cdot \text{kg} \cdot \text{m}^{-1} \cdot \text{sec}^{-1}$
$3.6787 \cdot 10^{-5} \cdot \text{kg} \cdot \text{m}^{-1} \cdot \text{sec}^{-1}$
$3.8194 \cdot 10^{-5} \cdot \text{kg} \cdot \text{m}^{-1} \cdot \text{sec}^{-1}$
$3.9573 \cdot 10^{-5} \cdot \text{kg} \cdot \text{m}^{-1} \cdot \text{sec}^{-1}$
$4.0926 \cdot 10^{-5} \cdot \text{kg} \cdot \text{m}^{-1} \cdot \text{sec}^{-1}$
$4.2254 \cdot 10^{-5} \cdot \text{kg} \cdot \text{m}^{-1} \cdot \text{sec}^{-1}$
$4.356 \cdot 10^{-5} \cdot \text{kg} \cdot \text{m}^{-1} \cdot \text{sec}^{-1}$
$4.4844 \cdot 10^{-5} \cdot \text{kg} \cdot \text{m}^{-1} \cdot \text{sec}^{-1}$
$4.6108 \cdot 10^{-5} \cdot \text{kg} \cdot \text{m}^{-1} \cdot \text{sec}^{-1}$

$$\mu_{\text{mix}}(T) := \exp\left(-0.6984944 + 0.640549 \cdot \ln\left(\frac{T}{K}\right) + \frac{-14.50559 \cdot K}{T}\right) \cdot 10^{-6} \cdot \text{kg} \cdot \text{m}^{-1} \cdot \text{sec}^{-1}$$

$$\mu_{\text{mix}}(1000 \cdot K) = 4.0926 \cdot 10^{-5} \cdot \text{kg} \cdot \text{m}^{-1} \cdot \text{sec}^{-1}$$

$$\mu_{\text{mix}}(1000 \cdot K) = 4.09256 \cdot 10^{-5} \cdot \text{kg} \cdot \text{m}^{-1} \cdot \text{sec}^{-1}$$

Define thermal conductivity functions for light molecules

$$\text{igas} := 0, 1..4$$

$$a\lambda := \begin{bmatrix} -1.869 \\ -0.3273 \\ 0.3919 \\ -7.215 \\ 7.341 \end{bmatrix} \quad b\lambda := \begin{bmatrix} 0.08727 \\ 0.09966 \\ 0.09816 \\ 0.08015 \\ -0.01013 \end{bmatrix} \quad c\lambda := \begin{bmatrix} 1.179 \cdot 10^{-4} \\ -(3.743 \cdot 10^{-5}) \\ -(5.067 \cdot 10^{-5}) \\ 5.477 \cdot 10^{-6} \\ 1.801 \cdot 10^{-4} \end{bmatrix}$$

$$d\lambda := \begin{bmatrix} -(3.614 \cdot 10^{-8}) \\ 9.732 \cdot 10^{-9} \\ 1.504 \cdot 10^{-8} \\ -(1.053 \cdot 10^{-8}) \\ -(9.1 \cdot 10^{-8}) \end{bmatrix}$$

CH4
O2
N2
CO2
H2O

$$\lambda(i, T) := \left[a\lambda_i + b\lambda_i \cdot \frac{T}{K} + c\lambda_i \cdot \left(\frac{T}{K}\right)^2 + d\lambda_i \cdot \left(\frac{T}{K}\right)^3 \right] \cdot 0.00001 \cdot \frac{W}{\text{cm} \cdot K}$$

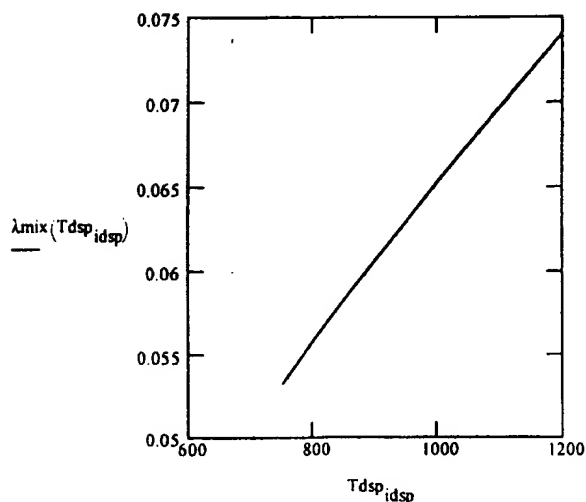
$$\lambda(\text{igas}, 1000 \cdot K)$$

0.16716 · kg · m · sec ⁻³ · K ⁻¹
0.07163 · kg · m · sec ⁻³ · K ⁻¹
0.06292 · kg · m · sec ⁻³ · K ⁻¹
0.06788 · kg · m · sec ⁻³ · K ⁻¹
0.08631 · kg · m · sec ⁻³ · K ⁻¹

W/m/K

$$\lambda_{\text{mix}}(T) := \sum_{i=1}^4 \frac{y_{eq_i} \cdot \lambda(i, T)}{\sum_{j=1}^4 y_{eq_j} \cdot \left[\frac{1 + \left(\frac{\mu(T)_i}{\mu(T)_j}\right)^{0.5} \cdot \left(\frac{MW_j}{MW_i}\right)^{0.25} \right]^2 \left[8 \cdot \left(1 + \frac{MW_i}{MW_j}\right) \right]^{0.5}}$$

$$\lambda_{\text{mix}}(1000 \cdot K) = 0.000653 \cdot \frac{W}{\text{cm} \cdot K}$$



$T_{\text{dsp_idsp}}$	$\lambda_{\text{mix}}(T_{\text{dsp_idsp}})$
$7.5 \cdot 10^2 \cdot K$	$0.05323 \cdot \text{kg} \cdot \text{m} \cdot \text{sec}^{-3} \cdot K^{-1}$
$8 \cdot 10^2 \cdot K$	$0.055775 \cdot \text{kg} \cdot \text{m} \cdot \text{sec}^{-3} \cdot K^{-1}$
$8.5 \cdot 10^2 \cdot K$	$0.058242 \cdot \text{kg} \cdot \text{m} \cdot \text{sec}^{-3} \cdot K^{-1}$
$9 \cdot 10^2 \cdot K$	$0.060641 \cdot \text{kg} \cdot \text{m} \cdot \text{sec}^{-3} \cdot K^{-1}$
$9.5 \cdot 10^2 \cdot K$	$0.06298 \cdot \text{kg} \cdot \text{m} \cdot \text{sec}^{-3} \cdot K^{-1}$
$1 \cdot 10^3 \cdot K$	$0.065268 \cdot \text{kg} \cdot \text{m} \cdot \text{sec}^{-3} \cdot K^{-1}$
$1.05 \cdot 10^3 \cdot K$	$0.067512 \cdot \text{kg} \cdot \text{m} \cdot \text{sec}^{-3} \cdot K^{-1}$
$1.1 \cdot 10^3 \cdot K$	$0.069721 \cdot \text{kg} \cdot \text{m} \cdot \text{sec}^{-3} \cdot K^{-1}$
$1.15 \cdot 10^3 \cdot K$	$0.071904 \cdot \text{kg} \cdot \text{m} \cdot \text{sec}^{-3} \cdot K^{-1}$
$1.2 \cdot 10^3 \cdot K$	$0.074069 \cdot \text{kg} \cdot \text{m} \cdot \text{sec}^{-3} \cdot K^{-1}$

$$\lambda_{\text{mix}}(T) := \exp\left[-7.073383 + 0.6397005 \cdot \ln\left(\frac{T}{K}\right) + \frac{-65.2387 \cdot K}{T}\right] \cdot W \cdot m^{-1} \cdot K^{-1}$$

$$\lambda_{\text{mix}}(1000 \cdot K) = 0.0653 \cdot m^{-1} \cdot K^{-1} \cdot W$$

$$\lambda_{\text{mix}}(1000 \cdot K) = 0.0659 \cdot m^{-1} \cdot K^{-1} \cdot W$$

Define heat capacities:

$$Cp_{\text{coef}} := \begin{bmatrix} 19.25 & .05213 & 0.00001197 & -0.00000001132 \\ 28.11 & -0.000368 & 0.00001746 & -0.00000001065 \\ 31.15 & -0.01357 & 0.0000268 & -0.00000001168 \\ 19.8 & 0.07344 & -0.00005602 & 0.00000001715 \\ 32.24 & 0.001924 & 0.00001055 & -0.000000003596 \\ 76.19 & 0.7867 & -0.0004204 & 0.00000007516 \end{bmatrix}$$

$$Cp(\text{igas}, T) := \sum_{jj=0}^3 Cp_{\text{coef}}_{\text{igas}, jj} \left(\frac{T}{K}\right)^{jj} \cdot \frac{J}{K}$$

J/mol/K

$$jj = 0..3$$

$$Cp(0, 300 \cdot K) = 35.6607 \cdot K^{-1} \cdot J$$

$$Cp(5, 300 \cdot K) = 124.0133 \cdot K^{-1} \cdot J$$

$$Cp_{\text{mix}}(T) := \sum_{jk=1}^4 Cp(jk, T) \cdot yeq_{jk}$$

$$Cp_{\text{mix}}(998 \cdot K) = 33.5144 \cdot J \cdot K^{-1}$$

$$Cp_{\text{cfmix}}_{jj} := \sum_{jk=1}^4 Cp_{\text{coef}}_{jk, jj} \cdot yeq_{jk} \cdot \frac{J}{K}$$

$$Cp_{\text{cfmix}} = \begin{bmatrix} 30.493459 \\ -0.009725 \\ 2.370305 \cdot 10^{-5} \\ -1.094786 \cdot 10^{-8} \end{bmatrix} \cdot \text{kg} \cdot \text{m}^2 \cdot \text{sec}^{-2} \cdot \text{K}^{-1}$$

$$Cp_{\text{mix}}(T) := \sum_{jj=0}^3 Cp_{\text{cfmix}}_{jj} \left(\frac{T}{K}\right)^{jj}$$

$$Cp_{\text{mix}}(1000 \cdot K) = 33.52413 \cdot \text{kg} \cdot \text{m}^2 \cdot \text{sec}^{-2} \cdot \text{K}^{-1}$$

$$Cp_{\text{mix}}(1000 \cdot K) = 33.52413 \cdot \text{kg} \cdot \text{m}^2 \cdot \text{sec}^{-2} \cdot \text{K}^{-1}$$

$$\text{igas} = 0, 1..6$$

$$P = 1.013 \cdot 10^5 \cdot \text{Pa}$$

Define momentum and thermal diffusivities:

$$\alpha(\text{igas}, T) := \frac{\lambda(\text{igas}, T) \cdot R \cdot T}{Cp(\text{igas}, T) \cdot P}$$

$$\alpha(0, 300 \cdot K) = 0.2344 \cdot \text{sec}^{-1} \cdot \text{cm}^2$$

$$\alpha_{\text{mix}}(T) := \frac{\lambda_{\text{mix}}(T) \cdot R \cdot T}{Cp_{\text{mix}}(T) \cdot P}$$

$$\alpha_{\text{mix}}(1000 \cdot K) = 1.6132 \cdot \text{sec}^{-1} \cdot \text{cm}^2$$

$$\nu_{\text{mix}}(T) := \frac{\mu_{\text{mix}}(T)}{\rho_{\text{mix}}(T)}$$

$$\nu_{\text{mix}}(1000 \cdot K) = 1.1732 \cdot \text{sec}^{-1} \cdot \text{cm}^2$$

$$\nu_{\text{mix}}(T) := \frac{\mu_{\text{mix}}(T)}{\rho_{\text{mix}}(T)}$$

$$\rho_{\text{mix}}(1000 \cdot K) = 3.48836 \cdot 10^{-4} \cdot \text{gm} \cdot \text{cm}^{-3}$$

$$\rho_{\text{mix}}(T) := \rho_{\text{mix}}(T)$$

$$D_{\text{ch4T}}(1000 \cdot K) = 1.7543 \cdot \text{sec}^{-1} \cdot \text{cm}^2$$

$$D_{\text{c7h14T}}(1000 \cdot K) = 0.5103 \cdot \text{sec}^{-1} \cdot \text{cm}^2$$

Define Prandtl, Schmidt, and Lewis numbers

$$Pr(T) := \frac{\nu_{\text{mix}}(T)}{\alpha_{\text{mix}}(T)}$$

$$Pr(1000 \cdot K) = 0.7272$$

$$Sc1T(T) := \frac{\nu_{\text{mix}}(T)}{D_{\text{ch4T}}(T)}$$

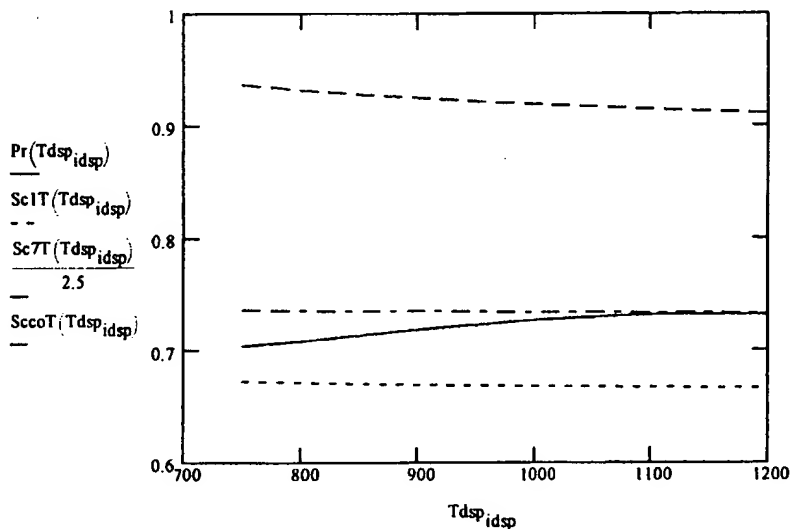
$$Sc1T(1000 \cdot K) = 0.6688$$

$$Sc7T(T) := \frac{\nu_{\text{mix}}(T)}{D_{\text{c7h14T}}(T)}$$

$$Sc7T(1000 \cdot K) = 2.299$$

$$SccoT(T) := \frac{\nu_{\text{mix}}(T)}{D_{\text{coT}}(T)}$$

$$SccoT(1000 \cdot K) = 0.7346$$



These relations have weak temperature dependence and (presumably) very weak dependence on composition

This ends the extended section that defines gas properties for the combustion mixtures.

Honeycombs: Represent as square channel metal alloy wall 0.003 mil, uncoated; 0.004 mil coated

$$dwalluc = 0.003 \cdot \text{in} \quad dwalluc = 7.62 \cdot 10^{-5} \cdot \text{m} \quad dwallc = 0.004 \cdot \text{in} \quad dwallc = 1.016 \cdot 10^{-4} \cdot \text{m}$$

$$Cells1 = 100 \cdot \text{in}^{-2} \quad dwall1 = dwallc \quad Cells2 = 200 \cdot \text{in}^{-2} \quad dwall2 = dwallc$$

$$dcell1 = (Cells1)^{-0.5} \cdot dwall1 \quad dcell2 = (Cells2)^{-0.5} \cdot dwall2$$

$$dcell1 = 0.2438 \cdot \text{cm} \quad ks1 = 0.002 \cdot \text{cm} \quad dcell2 = 0.1694 \cdot \text{cm} \quad ks2 = 0.002 \cdot \text{cm}$$

$$\epsilon_{cell1} = dcell1^2 \cdot Cells1 \quad \epsilon_{cell1} = 0.9216 \quad \epsilon_{cell2} = dcell2^2 \cdot Cells2 \quad \epsilon_{cell2} = 0.89006$$

$$Cells4 = 400 \cdot \text{in}^{-2} \quad dwall4 = dwallc$$

$$Cells6 = 600 \cdot \text{in}^{-2} \quad dwall6 = dwalluc$$

$$dcell4 = (Cells4)^{-0.5} \cdot dwall4 \quad dcell4 = 0.1168 \cdot \text{cm}$$

$$dcell6 = (Cells6)^{-0.5} \cdot dwall6 \quad dcell6 = 0.0961 \cdot \text{cm}$$

$$dcell4 = 0.1168 \cdot \text{cm} \quad ks4 = 0.001 \cdot \text{cm}$$

$$dcell6 = 0.0961 \cdot \text{cm} \quad ks6 = 0 \cdot \text{cm}$$

$$\epsilon_{cell4} = dcell4^2 \cdot Cells4 \quad \epsilon_{cell4} = 0.8464$$

$$\epsilon_{cell6} = dcell6^2 \cdot Cells6 \quad \epsilon_{cell6} = 0.85843$$

$$Cells8 = 800 \cdot \text{in}^{-2} \quad dwall8 = dwalluc$$

$$dcell8 = (Cells8)^{-0.5} \cdot dwall8 \quad dcell8 = 0.0822 \cdot \text{cm}$$

$$dcell8 = 0.0822 \cdot \text{cm} \quad ks8 = 0 \cdot \text{cm}$$

$$\epsilon_{cell8} = dcell8^2 \cdot Cells8 \quad \epsilon_{cell8} = 0.83749$$

Define recuperator and monolith configurations:

$$dreco = 17 \cdot \text{in}$$

$$dreco = 43.18 \cdot \text{cm}$$

$$Lrec = 7 \cdot \text{in}$$

$$dreci = 6 \cdot \text{in}$$

$$dreci = 15.24 \cdot \text{cm}$$

$$Lrec = 17.78 \cdot \text{cm}$$

$$\delta d = 1.375 \cdot \text{in}$$

Add space for mounting and insulation?

$$dhco = dreco - \delta d$$

$$dhco = 39.6875 \cdot \text{cm}$$

$$Lhc = 4 \cdot \text{in}$$

$$dhci = dreci + \delta d$$

$$dhci = 18.7325 \cdot \text{cm}$$

$$Lhc = 10.16 \cdot \text{cm}$$

$$Shc = \pi \cdot \frac{dhco^2 - dhci^2}{4}$$

$$Shc = 0.0961 \cdot \text{m}^2$$

$$Srecup = 0.0958 \cdot \text{m}^2$$

$$\frac{Srecup}{Shc} = 0.9964$$

Define initial combustion conditions

$$jcase = 0, 1 \dots 4$$

	0.2	1350	340
	0.26	1350	390
case	0.314	1350	440
	0.38	1350	490
	0.72	1190	675

Mass flow (lb/sec)
Recup T inlet (F)
Recup T outlet (F)

$$TKF(T) = \left(\frac{T}{K} - 273.15 \right) \cdot \frac{9}{5} + 32$$

$$TFK(t) = \frac{(t - 32) \cdot 5 \cdot K}{9} + 273.15 \cdot K$$

$$P_{rec} = 1 \cdot \text{atm}$$

$$P_{hc} = 1 \cdot \text{atm}$$

$$mf_{jcase+1} = case_{jcase,0} \cdot 0.454 \cdot \text{kg} \cdot \text{sec}^{-1}$$

$$T_{recin,jcase+1} = TFK(case_{jcase,1})$$

$$T_{recout,jcase+1} = TFK(case_{jcase,2})$$

$$mf = \begin{bmatrix} 0 \\ 0.0908 \\ 0.118 \\ 0.1426 \\ 0.1725 \\ 0.3269 \end{bmatrix} \cdot \text{kg} \cdot \text{sec}^{-1}$$

$$T_{recin} = \begin{bmatrix} 0 \\ 1005.37 \\ 1005.37 \\ 1005.37 \\ 1005.37 \\ 916.48 \end{bmatrix} \cdot \text{K}$$

$$T_{recout} = \begin{bmatrix} 0 \\ 444.26 \\ 472.04 \\ 499.82 \\ 527.59 \\ 630.37 \end{bmatrix} \cdot \text{K}$$

$$U_{rec,jcase+1} = \frac{mf_{jcase+1}}{\rho_{mix}(T_{recin,jcase+1}) \cdot \frac{S_{recup}}{2}}$$

$$U_{rec} = \begin{bmatrix} 0 \\ 5.4633 \\ 7.1023 \\ 8.5774 \\ 10.3803 \\ 17.929 \end{bmatrix} \cdot \text{m} \cdot \text{sec}^{-1}$$

$$G_{rec,jcase+1} = \frac{mf_{jcase+1}}{\left(\frac{S_{recup}}{2}\right)}$$

Only half of the recuperator cross section
is available for exhaust gas flow

$$U_{hc2,jcase+1} = \frac{mf_{jcase+1}}{\rho_{mix}(T_{recin,jcase+1}) \cdot Shc \cdot \epsilon_{cell2}}$$

$$U_{hc4,jcase+1} = U_{hc2,jcase+1} \cdot \frac{\epsilon_{cell2}}{\epsilon_{cell4}}$$

$$U_{hc6,jcase+1} = U_{hc2,jcase+1} \cdot \frac{\epsilon_{cell2}}{\epsilon_{cell6}}$$

$$U_{hc2} = \begin{bmatrix} 0 \\ 3.058 \\ 3.9753 \\ 4.801 \\ 5.8101 \\ 10.0353 \end{bmatrix} \cdot \text{m} \cdot \text{sec}^{-1}$$

$$U_{hc4} = \begin{bmatrix} 0 \\ 3.2157 \\ 4.1804 \\ 5.0487 \\ 6.1098 \\ 10.553 \end{bmatrix} \cdot \text{m} \cdot \text{sec}^{-1}$$

$$T_{avg} = \frac{T_{recin} + T_{recout}}{2}$$

$$T_{avg} = \begin{bmatrix} 0 \\ 724.8167 \\ 738.7056 \\ 752.5944 \\ 766.4833 \\ 773.4278 \end{bmatrix} \cdot \text{K}$$

Define average temperature etc/ for
estimated ΔP and ΔT in the recuperator

$$\rho_{mixrec}(T) = \frac{MW_{mix} \cdot P_{rec}}{R \cdot T}$$

$$\rho_{mixrec}(T_{avg}) = 0.4813 \cdot \text{kg} \cdot \text{m}^{-3}$$

Evaluate Reynolds numbers for use in calculating the momentum, heat, and mass transfer functions:

$$R_{rec6}(G, T) = \frac{G \cdot d_{cell6}}{\mu_{mix}(T)} \quad R_{rec6}(G_{rec1}, T_{avg1}) = 54.9906$$

$$R_{rec8}(G, T) = \frac{G \cdot d_{cell8}}{\mu_{mix}(T)} \quad R_{rec8}(G_{rec1}, T_{avg1}) = 47.0389$$

For laminar flow with entrance effect (adapted from Kays & Crawford, "Convective Heat and Mass Transfer"):

$$c_{frec8}(G, T, z) = \frac{14.227}{R_{rec8}(G, T)} \left[1 + 0.046263 \cdot \left(R_{rec8}(G, T) \cdot \frac{d_{cell8}}{z} \right)^{0.45363} \right]$$

Average coefficient of friction
for a smooth square channel

$$c_{frec6}(G, T, z) = \frac{14.227}{R_{rec6}(G, T)} \left[1 + 0.046263 \cdot \left(R_{rec6}(G, T) \cdot \frac{d_{cell6}}{z} \right)^{0.45363} \right]$$

Calculate monolith pressure drop in recuperator with entrance effect:

$$\Delta P_{rec8}_{jcase+1} = 4 \cdot c_{frec8}(G_{rec_{jcase+1}}, T_{avg_{jcase+1}}, L_{rec}) \cdot \frac{\left(\frac{U_{rec_{jcase+1}}}{2} \right)^2 \left[\rho_{mixrec}(T_{recin_{jcase+1}}) + \rho_{mixrec}(T_{recout_{jcase+1}}) \right] \left(\frac{T_{rec_{jcase+1}}}{T_{rec}} \right)}{2}$$

$$\Delta P_{rec6}_{jcase+1} = 4 \cdot c_{frec6}(G_{rec_{jcase+1}}, T_{avg_{jcase+1}}, L_{rec}) \cdot \frac{\left(\frac{U_{rec_{jcase+1}}}{2} \right)^2 \left[\rho_{mixrec}(T_{recin_{jcase+1}}) + \rho_{mixrec}(T_{recout_{jcase+1}}) \right] \left(\frac{T_{rec_{jcase+1}}}{T_{rec}} \right)}{2}$$

$$\frac{\Delta P_{rec8}}{Prec} = \begin{bmatrix} 0 \\ 0.0097 \\ 0.013 \\ 0.0162 \\ 0.0203 \\ 0.0393 \end{bmatrix}$$

$$\frac{\Delta P_{rec6}}{Prec} = \begin{bmatrix} 0 \\ 0.0071 \\ 0.0095 \\ 0.0119 \\ 0.0149 \\ 0.0289 \end{bmatrix}$$

$$\Delta P_{obs_P} = \begin{bmatrix} 0 \\ 0.011 \\ 0.014 \\ 0.018 \\ 0.022 \\ 0.042 \end{bmatrix}$$

Chose 800 cells per in2
with 10% length factor
in Lrec for chevrons

Averaged Nu for 800 cpi square channels (fully developed laminar flow) taken from Rosner:

$$\text{Nuhavgrec8}_{j\text{case}+1} = 2.976 \cdot \left[1 + \frac{7.6 \cdot (\text{Lrec} \cdot 1.1)}{\text{Rrec8}(\text{Grec}_{j\text{case}+1}, \text{Tavg}_{j\text{case}+1}) \cdot \text{Pr}(\text{Tavg}_{j\text{case}+1}) \cdot \text{dcell8}} \right]^{1/8}$$

$$\text{Nuhavgrec8} = \begin{bmatrix} 0 \\ 2.976 \\ 2.976 \\ 2.976 \\ 2.976 \\ 2.9762 \end{bmatrix}$$

Entrance effect for heat transfer within the recuperator is only significant for the first half inch - average Nusselt No. = 2.976 for all cases

$$\text{hrecavg}_{j\text{case}+1} = \frac{\lambda_{\text{mix}}(\text{Tavg}_{j\text{case}+1}) \cdot \text{Nuhavgrec8}_{j\text{case}+1}}{\text{dcell8}}$$

$$\text{hrecavg} = \begin{bmatrix} 0 \\ 188.0022 \\ 190.6356 \\ 193.2448 \\ 195.8307 \\ 197.1273 \end{bmatrix} \cdot \text{kg} \cdot \text{sec}^{-3} \cdot \text{K}^{-1}$$

W/m2/K

$$\Delta T_{\text{skin}, j\text{case}+1} = \frac{\text{Grec}_{j\text{case}+1} \cdot \text{dcell8} \cdot (\text{Cpmix}(\text{Trecout}_{j\text{case}+1}) \cdot \text{Trecout}_{j\text{case}+1} - \text{Cpmix}(\text{Trecin}_{j\text{case}+1}) \cdot \text{Trecin}_{j\text{case}+1})}{\text{MWmix} \cdot \text{hrecavg}_{j\text{case}+1} \cdot 4 \cdot \text{Lrec} \cdot 1.1}$$

$$\Delta T_{\text{skin}} = \begin{bmatrix} 0 \\ -7.5657 \\ -9.274 \\ -10.5339 \\ -11.9549 \\ -13.635 \end{bmatrix} \cdot \text{K}$$

$$\Delta T_{\text{skin}} \cdot 2 \cdot \frac{9}{5 \cdot \text{K}} = \begin{bmatrix} 0 \\ -27.2364 \\ -33.3864 \\ -37.9221 \\ -43.0378 \\ -49.0859 \end{bmatrix}$$

Approximate average ΔT (F)
across wall in recuperator

ΔT seems low - more conservative calculation uses dcell for 600 cells/in2 - in this case ΔT maximum increases from 50F to about 70F

$$\Delta T_{\text{skin}} \cdot 2 \cdot \frac{9}{5 \cdot \text{K}} \cdot \left(\frac{\text{dcell6}}{\text{dcell8}} \right)^2 = \begin{bmatrix} 0 \\ 37.2231 \\ 45.628 \\ 51.8268 \\ 58.8182 \\ 67.0839 \end{bmatrix}$$

$$\left(\frac{\text{dcell6}}{\text{dcell8}} \right)^2 = 1.3667$$

Use 600 cells/in² in recuperator dimension for conservative calculation of CH₄, C₇H₁₄, and CO conversions

Find mass transfer rates via Nusselt formulas:

$$\text{Numavgrec6cl}_{j\text{case}+1} = 2.976 \cdot \left[1 + \left(\frac{7.6 \cdot \text{Lrec} \cdot 1.1}{\text{Rerec6}(\text{Grec}_{j\text{case}+1}, \text{Tavg}_{j\text{case}+1}) \cdot \text{Sc1T}(\text{Tavg}_{j\text{case}+1}) \cdot \text{dcell6}} \right)^{\frac{8}{3}} \right]^{\frac{1}{8}} \quad \text{Numavgrec6cl} = \begin{bmatrix} 0 \\ 2.976 \\ 2.976 \\ 2.9761 \\ 2.9761 \\ 2.9765 \\ 0 \\ 2.9765 \\ 2.977 \\ 2.9775 \\ 2.9784 \\ 2.9891 \end{bmatrix}$$

$$\text{Numavgrec6c7}_{j\text{case}+1} = 2.976 \cdot \left[1 + \left(\frac{7.6 \cdot \text{Lrec} \cdot 1.1}{\text{Rerec6}(\text{Grec}_{j\text{case}+1}, \text{Tavg}_{j\text{case}+1}) \cdot \text{Sc7T}(\text{Tavg}_{j\text{case}+1}) \cdot \text{dcell6}} \right)^{\frac{8}{3}} \right]^{\frac{1}{8}} \quad \text{Numavgrec6c7} = \begin{bmatrix} 0 \\ 2.9765 \\ 2.977 \\ 2.9775 \\ 2.9784 \\ 2.9891 \end{bmatrix}$$

$$\text{Numavgrec6co}_{j\text{case}+1} = 2.976 \cdot \left[1 + \left(\frac{7.6 \cdot \text{Lrec} \cdot 1.1}{\text{Rerec6}(\text{Grec}_{j\text{case}+1}, \text{Tavg}_{j\text{case}+1}) \cdot \text{SccoT}(\text{Tavg}_{j\text{case}+1}) \cdot \text{dcell6}} \right)^{\frac{8}{3}} \right]^{\frac{1}{8}} \quad \text{Numavgrec6co} = \begin{bmatrix} 0 \\ 2.976 \\ 2.976 \\ 2.9761 \\ 2.9761 \\ 2.9766 \end{bmatrix}$$

Once again the entrance effects within the recuperator are negligible

The average (integral) Nusselt numbers at 1-atm show very little contribution of the thermal entry length, i.e. the flow velocities and heat and mass transfer coefficients have values close to those in long channels.

Now determine the maximum possible CH₄, C₇H₁₄, and CO conversions in a 600 cells per in² recuperator

$$\text{ych40} = 0.005$$

$$\text{yc7h140} = 0.0005$$

$$\text{yco0} = 0.005$$

Start with maximum concentrations of added pollutants

$$\text{ych4rec6}_{j\text{case}+1} = \text{ych40} \cdot \exp \left(\frac{-4 \cdot \text{Lrec} \cdot 1.1 \cdot \text{Numavgrec6cl}_{j\text{case}+1}}{\text{Rerec6}(\text{Grec}_{j\text{case}+1}, \text{Tavg}_{j\text{case}+1}) \cdot \text{Sc1T}(\text{Tavg}_{j\text{case}+1}) \cdot \text{dcell6}} \right)$$

$$\frac{-4 \cdot \text{Lrec} \cdot 1.1 \cdot \text{Numavgrec6cl}_{j\text{case}+1}}{\text{Rerec6}(\text{Grec}_{j\text{case}+1}, \text{Tavg}_{j\text{case}+1}) \cdot \text{Sc1T}(\text{Tavg}_{j\text{case}+1}) \cdot \text{dcell6}}$$

65.4083
50.9771
42.7552
35.7764
19.0017

$$\frac{\text{ych4rec6}}{\text{ych40}} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 5.5932 \cdot 10^{-9} \end{bmatrix}$$

$$yc7h14rec6_{jcase+1} = yc7h140 \cdot \exp\left(\frac{-4 \cdot Lrec \cdot 1.1 \cdot Numavgrec6c7_{jcase+1}}{Rerec6(Grec_{jcase+1}, Tavg_{jcase+1}) \cdot Sc7T(Tavg_{jcase+1}) \cdot dcell6}\right)$$

$yc7h14rec6 = \begin{bmatrix} 0 \\ 3.5287 \cdot 10^{-12} \\ 2.1834 \cdot 10^{-10} \\ 2.2859 \cdot 10^{-9} \\ 1.6805 \cdot 10^{-8} \\ 2.0597 \cdot 10^{-6} \end{bmatrix}$	$\frac{yc7h14rec6}{yc7h140} = \begin{bmatrix} 0 \\ 7.057 \cdot 10^{-9} \\ 4.367 \cdot 10^{-7} \\ 4.572 \cdot 10^{-6} \\ 3.361 \cdot 10^{-5} \\ 4.119 \cdot 10^{-3} \end{bmatrix}$	$\frac{-4 \cdot Lrec \cdot 1.1 \cdot Numavgrec6c7_{jcase+1}}{Rerec6(Grec_{jcase+1}, Tavg_{jcase+1}) \cdot Sc7T(Tavg_{jcase+1}) \cdot dcell6}$ <table border="1"> <tr><td>-18.7692</td></tr> <tr><td>-14.6441</td></tr> <tr><td>-12.2956</td></tr> <tr><td>-10.3007</td></tr> <tr><td>-5.492</td></tr> </table>	-18.7692	-14.6441	-12.2956	-10.3007	-5.492
-18.7692							
-14.6441							
-12.2956							
-10.3007							
-5.492							

$$ycorec6_{jcase+1} = yco0 \cdot \exp\left(\frac{-4 \cdot Lrec \cdot 1.1 \cdot Numavgrec6co_{jcase+1}}{Rerec6(Grec_{jcase+1}, Tavg_{jcase+1}) \cdot ScCoT(Tavg_{jcase+1}) \cdot dcell6}\right)$$

$ycorec6 = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1.457 \cdot 10^{-10} \end{bmatrix}$	$\frac{ycorec6}{yco0} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 6.4676 \cdot 10^{-15} \\ 2.914 \cdot 10^{-8} \end{bmatrix}$	$\frac{-4 \cdot Lrec \cdot 1.1 \cdot Numavgrec6co_{jcase+1}}{Rerec6(Grec_{jcase+1}, Tavg_{jcase+1}) \cdot ScCoT(Tavg_{jcase+1}) \cdot dcell6}$ <table border="1"> <tr><td>-59.7854</td></tr> <tr><td>-46.5803</td></tr> <tr><td>-39.0561</td></tr> <tr><td>-32.672</td></tr> <tr><td>-17.3512</td></tr> </table>	-59.7854	-46.5803	-39.0561	-32.672	-17.3512
-59.7854							
-46.5803							
-39.0561							
-32.672							
-17.3512							

00033663-0822001

With 5000ppm C7H14 in turbine exhaust, exit concentration reaches 20 ppm at the highest power level for conservative 600 cells/in² calculation. For 800 cells/in², the exit concentration in this case would reach about 2 ppm. With only 500ppm C7H14 in the inlet, should get <2 ppm in the outlet of the recuperator assuming favorable catalytic rates at the wall. Also this calculation used averaged temperature and flow conditions - will compare below a 1-dimensional (axial) calculation that determines the effect of decreasing temperature on the kinetics and mass transport.

Maximum possible (transport-limited) CO and CH₄ conversions in a 7 in. 600-800 cells/in² recuperator are >99.99%, while cyclohexane conversion is >99.6%. The final CO and C7H14 levels are < 1 ppb and .2 ppm for post turbine concentrations of 1000 and 50 ppm, respectively.

An alternative method of calculating performance uses local Nusselt numbers for heat and mass transfer to determine the wall temperature and combustion rates at the wall. First we define the local Nu function then check conversion assuming fast kinetics and compare with the previous averaged (integrated) Nu formula.

Local Nu(x) taken from Kays & Crawford for hydro & thermal laminar flow entrance with circular channel (modified for square channel by a factor 2.96/3.66:

ncase = 5

$$\text{Numono}(z) := (1 + \exp(-1.09689 - 0.381402 \cdot \ln(z) - 8.287774 \cdot z^{0.5})) \cdot 2.976 \quad \text{Numono}(0.1152163) = 3.112$$

$$\text{zzchar6c7}_{j\text{case}+1} := \frac{\text{Rrec6}(\text{Grec}_{j\text{case}+1}, \text{Trecin}_{j\text{case}+1}) \cdot \text{Sc7T}(\text{Trecin}_{j\text{case}+1}) \cdot \text{dcell6}}{2}$$

$$\frac{\text{Lrec}}{\text{zzchar6c7}_{\text{ncase}}} = 0.9444$$

Case specific

$$\text{zzchar6c1}_{j\text{case}+1} := \frac{\text{Rrec6}(\text{Grec}_{j\text{case}+1}, \text{Trecin}_{j\text{case}+1}) \cdot \text{Sc1T}(\text{Trecin}_{j\text{case}+1}) \cdot \text{dcell6}}{2}$$

$$\frac{\text{Lrec}}{\text{zzchar6c1}_{\text{ncase}}} = 3.2574$$

Case specific

$$\text{nz} := 400$$

$$\text{iz} := 0..nz$$

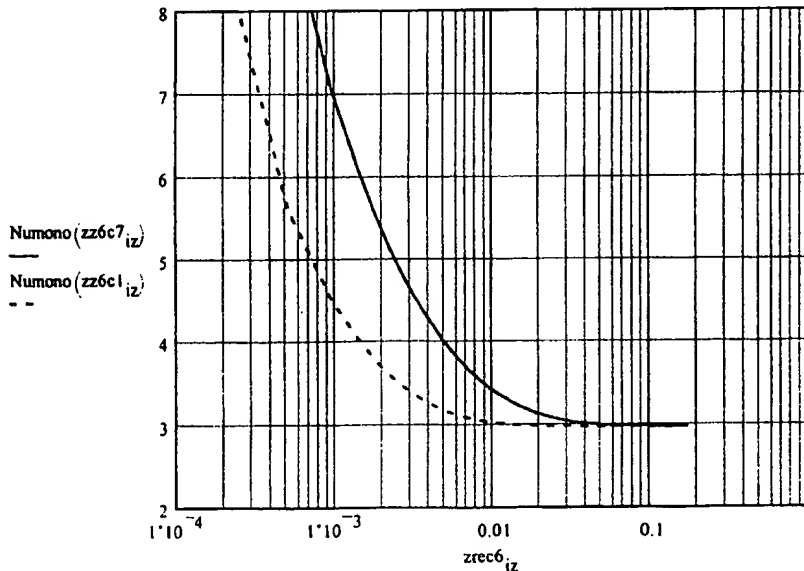
$$\text{Lrec} = 17.78 \text{ cm} \quad \text{dcell6} = 0.0961 \text{ cm}$$

$$\text{zrec6}_{\text{iz}} := \text{iz} \cdot \frac{\text{Lrec}}{\text{nz}} + \text{dwall6}$$

$$\text{zz6c7}_{\text{iz}} := \frac{\text{zrec6}_{\text{iz}}}{\text{zzchar6c7}_{\text{ncase}}} \quad \text{zz6c1}_{\text{iz}} := \frac{\text{zrec6}_{\text{iz}}}{\text{zzchar6c1}_{\text{ncase}}}$$

$$\text{zzchar6c7} = \begin{bmatrix} 0 \\ 4.896 \\ 6.3647 \\ 7.6867 \\ 9.3023 \\ 18.8265 \end{bmatrix} \text{ cm}$$

$$\text{zzchar6c1} = \begin{bmatrix} 0 \\ 1.4244 \\ 1.8518 \\ 2.2364 \\ 2.7064 \\ 5.4583 \end{bmatrix} \text{ cm}$$



Case specific ncase = 5

Case specific ncase = 5

$$\text{kgpbl6c7}(T, z) = \frac{\text{Dc7h14T}(T) \cdot \text{Numono} \left(\frac{z}{\text{zzchar6c7}_{\text{ncase}}} \right)}{\text{dcell6}}$$

$$\text{kgpbl6c7}(\text{Trecin}_{\text{ncase}}, \text{Lrec}) = 13.6159 \cdot \text{sec}^{-1} \cdot \text{cm}$$

$$\text{kgpbl6c1}(T, z) = \frac{\text{Dch4T}(T) \cdot \text{Numono} \left(\frac{z}{\text{zzchar6c1}_{\text{ncase}}} \right)}{\text{dcell6}}$$

$$\text{kgpbl6c1}(\text{Trecin}_{\text{ncase}}, \text{Lrec}) = 46.9581 \cdot \text{sec}^{-1} \cdot \text{cm}$$

$$\text{Trecz}_{\text{iz}} = \text{Trecin}_{\text{ncase}} - \frac{\text{Trecin}_{\text{ncase}} - \text{Trecout}_{\text{ncase}}}{\text{nz}} \cdot \text{iz}$$

$$\text{Trecz}_{\text{nz}} = 630.3722 \cdot \text{K}$$

$$\text{Trecout}_{\text{ncase}} = 630.3722 \cdot \text{K}$$

Determine maximum conversion of fuels with very fast catalytic combustion rates (zero fuel concentration at the wall)

$$\text{yzc7h14}_0 = \text{yc7h140}$$

$$\text{yzch4}_0 = \text{ych40}$$

ncase = 5

$$\text{yzc7h14}_{\text{iz}+1} = \left(1 - \text{kgpbl6c7}(\text{Trecz}_{\text{iz}}, \text{zrec6}_{\text{iz}}) \cdot \frac{\text{Lrec}}{\text{nz}} \cdot 1.1 \cdot \frac{4}{\text{dcell6}} \cdot \frac{\text{ecell6}}{\text{Urec}_{\text{ncase}}} \cdot \frac{\text{Trecin}_{\text{ncase}}}{\text{Trecz}_{\text{iz}}} \right) \cdot \text{yzc7h14}_{\text{iz}}$$

Case specific

$$\text{yzch4}_{\text{iz}+1} = \left(1 - \text{kgpbl6c1}(\text{Trecz}_{\text{iz}}, \text{zrec6}_{\text{iz}}) \cdot \frac{\text{Lrec}}{\text{nz}} \cdot 1.1 \cdot \frac{4}{\text{dcell6}} \cdot \frac{\text{ecell6}}{\text{Urec}_{\text{ncase}}} \cdot \frac{\text{Trecin}_{\text{ncase}}}{\text{Trecz}_{\text{iz}}} \right) \cdot \text{yzch4}_{\text{iz}}$$

Case specific

$$\text{yzc7h14}_{\text{nz}} = 3.385 \cdot 10^{-6}$$

$$\text{yzc7h14}_0 = 0.0005$$

$$\frac{\text{yzc7h14}_{\text{nz}}}{\text{yzc7h14}_0} = 6.77 \cdot 10^{-3}$$

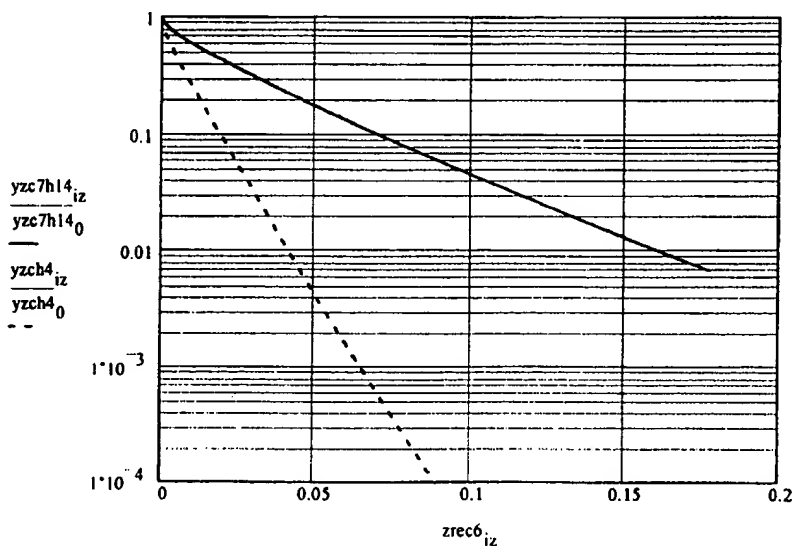
$$\frac{\text{yzch4}_{\text{nz}}}{\text{yzch4}_0} = 4.3292 \cdot 10^{-8}$$

$$\text{yzch4}_{\text{nz}} = 2.1646 \cdot 10^{-10}$$

$$\text{yzch4}_0 = 0.005$$

$$\frac{\text{yzc7h14}_{\text{nz}}}{\text{yzc7h14}_0} = 6.77 \cdot 10^{-3}$$

$$\frac{\text{yzch4}_{\text{nz}}}{\text{yzch4}_0} = 4.3292 \cdot 10^{-8}$$



Conversion of C7H14 under case 5 (full power) is 99.3% [vs. 99.6% via averaged integrated formulas] with about 1 inch entry length. Conversion of CH4 (and also CO) is very high (>99.99%) within 3.5 inches.

This result shows that the averaged integrated values for CH4, C7H14, and CO conversions are very good approximations and can be used for different values of fuel and CO concentrations.

Case specific ncase = 5

 Add finite rate kinetics for PdO/Al₂O₃ methane combustion catalyst
 Begin by defining a few constants and catalyst functions

$$R = 82.076 \cdot K^{-1} \cdot atm \cdot cm^3 \quad atm \cdot cm^3 / mol \cdot K$$

$$R_{cm} := 83143000 \cdot gm \cdot cm^2 \cdot sec^{-2} \cdot K^{-1} \quad TOL := 0.0001$$

Define Catalyst Functions:

$$\eta_{sph}(\phi) := \frac{3}{\phi} \left(\frac{1}{\tanh(\phi)} - \frac{1}{\phi} \right)$$

$$\eta_{fpl}(\phi) := \frac{\tanh(\phi)}{\phi}$$

Catalyst Physical Properties for Pd/Al₂O₃

$$Scat := 85 \cdot m^2 \cdot gm^{-1} \quad \rho_{catpart} := 2.5 \cdot gm \cdot cm^{-3}$$

$$V_{\mu pore} := 0.15 \cdot cm^3 \cdot gm^{-1} \quad d_{pcat} := 0.0002 \cdot cm$$

$$L_{cat} := 0.0020 \cdot cm$$

$$d_{\mu pore} := 6 \cdot \frac{V_{\mu pore}}{Scat} \quad \epsilon_{\mu pore} := 0.375 \quad \tau_{\mu pore} := 3.0$$

$$d_{\mu pore} = 1.0588 \cdot 10^{-6} \cdot cm$$

$$DeffCH4(T) := \frac{\epsilon_{\mu pore}}{\tau_{\mu pore}} \left(\frac{1}{Dch4T(T)} + \frac{3}{d_{\mu pore} \cdot \sqrt{\frac{8 \cdot R \cdot T}{\pi \cdot MW_0}}} \right)$$

$$d_{\mu pore} \cdot \sqrt{\frac{8 \cdot R \cdot T_{in}}{\pi \cdot MW_0}} = 0.1095 \cdot sec^{-1} \cdot cm^2$$

$$DeffCH4(T_{in}) = 4.43271 \cdot 10^{-3} \cdot sec^{-1} \cdot cm^2$$

$$Dch4T(T_{in}) = 1.2343 \cdot sec^{-1} \cdot cm^2$$

$$d_{\text{pore}} \cdot \frac{\pi \cdot R \cdot T \cdot \ln}{MW_6} = 0.0829 \cdot \text{sec}^{-1} \cdot \text{cm}^2$$

$$D_{c7h14}(T_{in}) = 0.356 \cdot \text{sec}^{-1} \cdot \text{cm}^2$$

$$D_{\text{macCH4}}(800\text{-K}) = 0.193 \cdot \text{sec}^{-1} \cdot \text{cm}^2$$

$$D_{\text{macC7H14}}(800\cdot\text{K}) = 0.0556\cdot\text{sec}^{-1}\cdot\text{cm}^2$$

Test value for kOT

Questions **A**nswers **E**xercises

$$\phi_{\mu}(k0T, T_{in}) = 0.2042$$

$$\Phi_{\text{mac}}(k_0 T, T_{\text{in}}) = 1.8333$$
$$\phi_{\mu 7}(k_0 T, T_{in}) = 0.2402$$
$$\Phi_{\text{mac7}}(k_0T, T_{\text{in}}) = 3.4117$$

$$\text{RatekCH4}(k_0T, T_{in}) = 85999.4914 \cdot \text{sec}^{-1}$$

$$\text{Rate}_{\text{C7H14}}(\text{kOT}, T_{\text{in}}) = 48479.296 \cdot \text{sec}^{-1}$$

Defines transport restricted rate constant function given catalyst effective first order rate constant, k_0T , methane or cyclohexane concentration, x , and surface temperature, T

PdO Catalyst Rate Constants

$$\text{Erpd0} := 12800 \cdot \text{K} \quad \text{Erpd1} := 4900 \cdot \text{K} \quad \text{Erpd3} := 15000 \cdot \text{K}$$

Region0 - low T PdO to 625K
ignores inhibition by H₂O and CO₂

Region1 - Intermediate T
625K to 909K

Region2 - Flat 909K
to 1048K decomposition

Region3 -
Pd metal

$$\text{Apd0} := 2.4 \cdot 10^3 \cdot 200 \cdot \text{gm}^{-1} \cdot \text{sec}^{-1}$$

$$\text{Apd1} := \text{Apd0} \cdot \exp\left(-\frac{\text{Erpd0}}{625 \cdot \text{K}} + \frac{\text{Erpd1}}{625 \cdot \text{K}}\right)$$

$$\text{Apd2} := \text{Apd1} \cdot \exp\left(\frac{-\text{Erpd1}}{909.1 \cdot \text{K}}\right)$$

$$\text{Apd3} := \text{Apd2} \cdot \exp\left(\frac{\text{Erpd3}}{1048.1 \cdot \text{K}}\right)$$

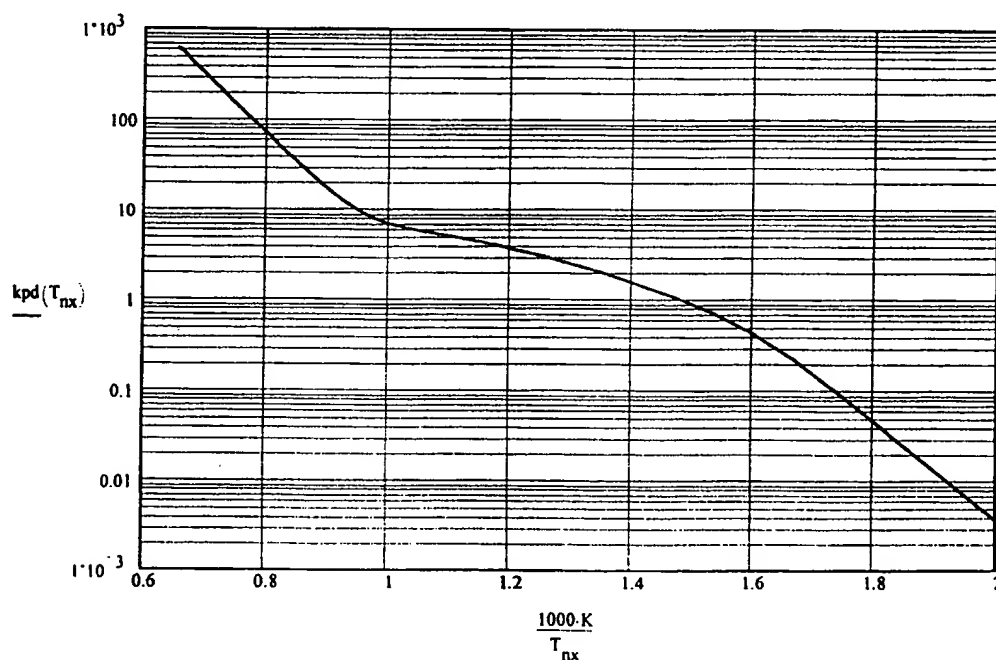
Interpolation formula for the four PdO+Pd rate constants

$$k_{pd}(T) := \left[\text{Apd3}^2 \cdot \exp\left(-\frac{2 \cdot \text{Erpd3}}{T}\right) + \frac{1}{\left(\text{Apd2}^{-2} + \text{Apd1}^{-2} \cdot \exp\left(\frac{2 \cdot \text{Erpd1}}{T}\right) + \text{Apd0}^{-2} \cdot \exp\left(\frac{2 \cdot \text{Erpd0}}{T}\right) \right)} \right]^{0.5}$$

$$n_x := 0, 1 \dots 41$$

$$T_{nx} := 500 \cdot \text{K} + n_x \cdot 25 \cdot \text{K}$$

CATALYTIC RATE CONSTANT vs TEMPERATURE (mol/atmCH₄/s/gcat)

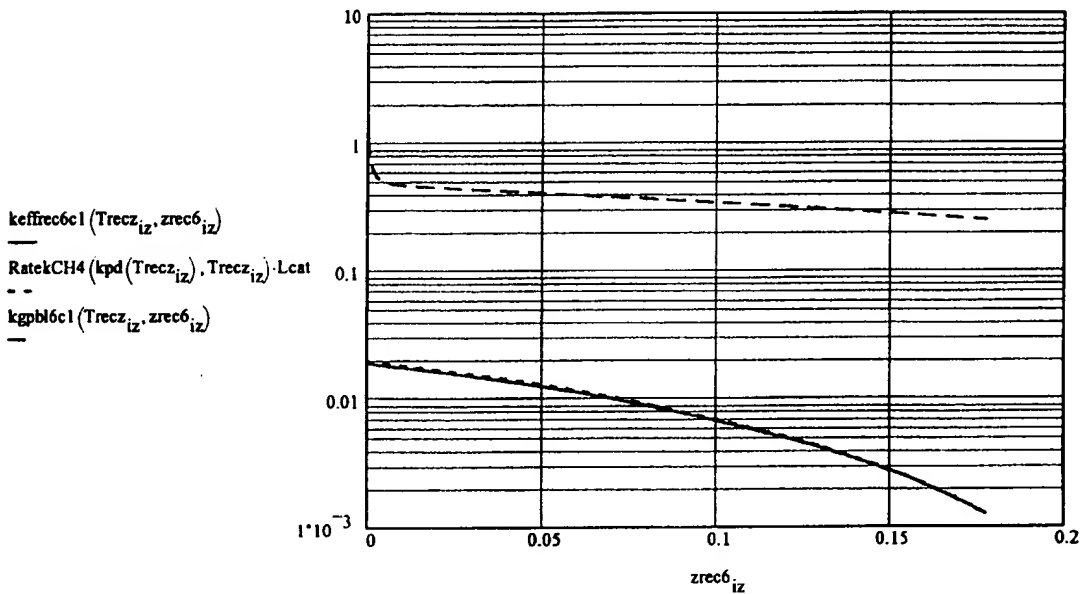


$$\text{keffrec6c1}(T, z) = \frac{1}{\left(\frac{1}{\text{RatekCH4}(\text{kpd}(T), T) \cdot \text{Lcat}} \right) + \text{kgpbl6c1}(T, z)} \quad \text{kgpbl6c1}\left(\text{Tavg}_{\text{ncase}}, \frac{\text{Lrec}}{2}\right) = 35.3023 \cdot \text{sec}^{-1} \cdot \text{cm}$$

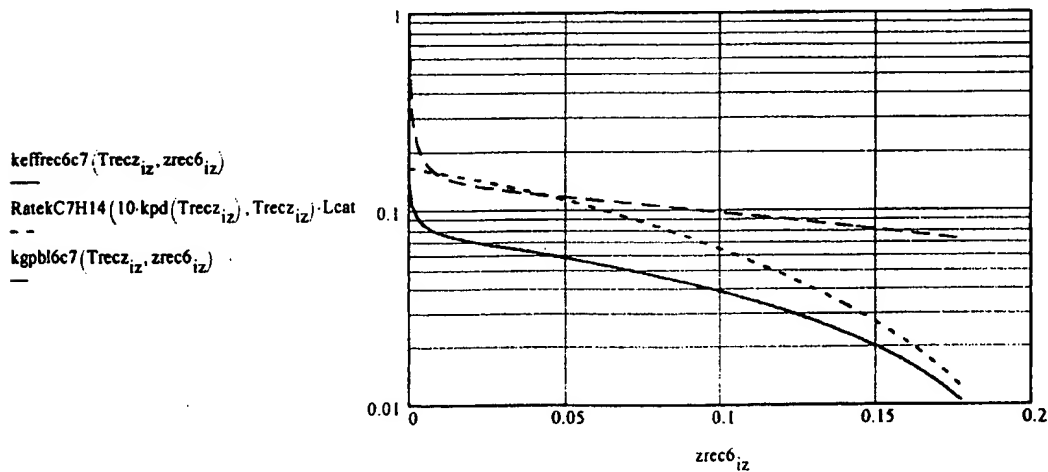
$$\text{keffrec6c1}\left(\text{Tavg}_{\text{ncase}}, \frac{\text{Lrec}}{2}\right) = 0.7922 \cdot \text{sec}^{-1} \cdot \text{cm} \quad \text{RatekCH4}\left(\text{kpd}(\text{Tavg}_{\text{ncase}}), \text{Tavg}_{\text{ncase}}\right) \cdot \text{Lcat} = 0.8104 \cdot \text{sec}^{-1} \cdot \text{cm}$$

$$\text{keffrec6c7}(T, z) = \frac{1}{\left(\frac{1}{\text{RatekC7H14}(10 \cdot \text{kpd}(T), T) \cdot \text{Lcat}} \right) + \text{kgpbl6c7}(T, z)} \quad \text{kgpbl6c7}\left(\text{Tavg}_{\text{ncase}}, \frac{\text{Lrec}}{2}\right) = 10.1756 \cdot \text{sec}^{-1} \cdot \text{cm}$$

$$\text{keffrec6c7}\left(\text{Tavg}_{\text{ncase}}, \frac{\text{Lrec}}{2}\right) = 4.2778 \cdot \text{sec}^{-1} \cdot \text{cm} \quad \text{RatekC7H14}\left(10 \cdot \text{kpd}(\text{Tavg}_{\text{ncase}}), \text{Tavg}_{\text{ncase}}\right) \cdot \text{Lcat} = 7.3807 \cdot \text{sec}^{-1} \cdot \text{cm}$$



Case specific ncase = 5



Determine conversion of fuels with transport-limited finite catalytic combustion rates:

Case specific $n_{case} = 5$

$$Trec_{iz} = Trec_{n_{case}} - \frac{Trec_{n_{case}} - Trec_{out_{n_{case}}}}{nz} \cdot iz$$

$$Trec_{nz} = 630.3722 \cdot K$$

$$Trec_{out_{n_{case}}} = 630.3722 \cdot K$$

$$yzkc7h14_0 = yz7h140$$

$$yzkch4_0 = ych40$$

$$yzkc7h14_{iz+1} = \left(1 - keffrec6c7(Trec_{iz}, zrec6_{iz}) \cdot \frac{Lrec}{nz} \cdot 1.1 \cdot \frac{4}{dcell6} \cdot \frac{\epsilon_{cell6}}{Urec_{n_{case}}} \cdot \frac{Trec_{iz}}{Trec_{nz}} \right) \cdot yzkc7h14_{iz}$$

Case specific

$n_{case} = 5$

$$yzkch4_{iz+1} = \left(1 - keffrec6c1(Trec_{iz}, zrec6_{iz}) \cdot \frac{Lrec}{nz} \cdot 1.1 \cdot \frac{4}{dcell6} \cdot \frac{\epsilon_{cell6}}{Urec_{n_{case}}} \cdot \frac{Trec_{iz}}{Trec_{nz}} \right) \cdot yzkch4_{iz}$$

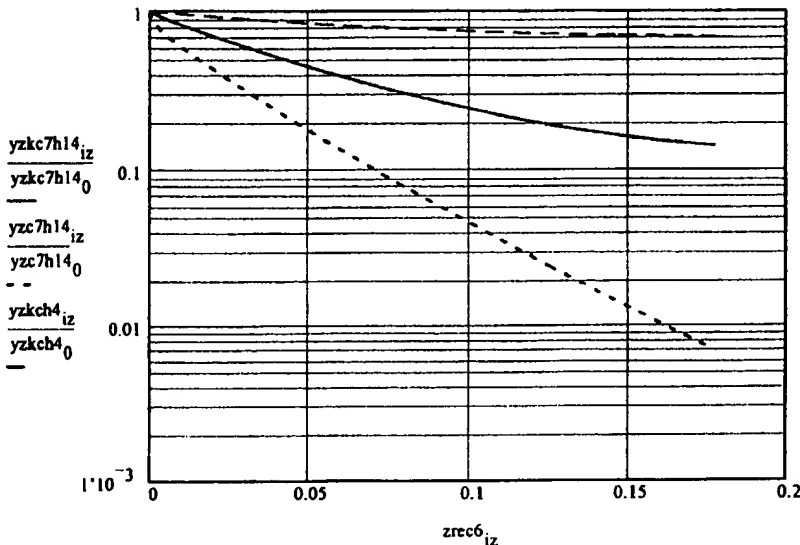
Case specific

$$\begin{aligned} yzkc7h14_{nz} &= 7.036 \cdot 10^{-5} & yzkc7h14_0 &= 0.0005 & \frac{yzkc7h14_{nz}}{yzkc7h14_0} &= 1.407 \cdot 10^{-1} & \frac{yzkch4_{nz}}{yzkch4_0} &= 0.6838 \\ yzkch4_{nz} &= 0.0034 & yzkch4_0 &= 0.005 \end{aligned}$$

Case specific $n_{case} = 5$

Conversion of C7H14 under case 5 (full power) is 99.4% [vs. 99.3% for the maximum BL transport-limited conversion] with gradually decreasing (rate limited) conversion. Conversion of CH4 is very poor (35%). CO conversion is probably very high given higher catalytic and transport rates than with C7H14.

This result shows that the specific rates of catalytic oxidation of all added components needs to be measured as applied to a recuperator. The use of a recuperator for emission control would appear to be greatly enhanced with higher exhaust (recuperator) temperatures.



In the following section, the conversion of C7H14, CH4 and CO is considered for various honeycomb monoliths

$$Thc_{jcase+1} = Trecin_{jcase+1}$$

$$\rho_{mixhc}_{jcase+1} = \rho_{mixrec}(Trecin_{jcase+1})$$

$$Ghc2_{jcase+1} = \frac{mf_{jcase+1}}{Shc \cdot dcell2}$$

$$Ghc4_{jcase+1} = \frac{mf_{jcase+1}}{Shc \cdot dcell4}$$

$$Ghc6_{jcase+1} = \frac{mf_{jcase+1}}{Shc \cdot dcell6}$$

$$Uhc2 = \begin{bmatrix} 0 \\ 3.058 \\ 3.9753 \\ 4.801 \\ 5.8101 \\ 10.0353 \end{bmatrix} \cdot m \cdot sec^{-1}$$

$$Uhc4 = \begin{bmatrix} 0 \\ 3.2157 \\ 4.1804 \\ 5.0487 \\ 6.1098 \\ 10.553 \end{bmatrix} \cdot m \cdot sec^{-1}$$

$$Uhc6 = \begin{bmatrix} 0 \\ 3.1706 \\ 4.1218 \\ 4.9779 \\ 6.0242 \\ 10.4051 \end{bmatrix} \cdot m \cdot sec^{-1}$$

Evaluate Reynolds numbers for use in calculating the momentum, heat, and mass transfer functions:

$$Rehc2_{jcase+1} = \frac{Ghc2_{jcase+1} \cdot dcell2}{\mu_{mixT}(Thc_{jcase+1})}$$

$$Rehc4_{jcase+1} = \frac{Ghc4_{jcase+1} \cdot dcell4}{\mu_{mixT}(Thc_{jcase+1})}$$

$$Rehc6_{jcase+1} = \frac{Ghc6_{jcase+1} \cdot dcell6}{\mu_{mixT}(Thc_{jcase+1})}$$

$$Rehc2 = \begin{bmatrix} 0 \\ 43.776 \\ 56.9088 \\ 68.7283 \\ 83.1744 \\ 167.4548 \end{bmatrix}$$

$$Rehc4 = \begin{bmatrix} 0 \\ 31.7427 \\ 41.2655 \\ 49.836 \\ 60.3111 \\ 121.4242 \end{bmatrix}$$

$$Rehc6 = \begin{bmatrix} 0 \\ 25.7355 \\ 33.4562 \\ 40.4048 \\ 48.8975 \\ 98.4453 \end{bmatrix}$$

$$cfrihc2(j,z) = \frac{14.227}{Rehc2_j} \left[1 + 0.046263 \cdot \left(Rehc2_j \cdot \frac{dcell2}{z} \right) \right]^{0.45363}$$

$$cfrihc4(j,z) = \frac{14.227}{Rehc4_j} \left[1 + 0.046263 \cdot \left(Rehc4_j \cdot \frac{dcell4}{z} \right) \right]^{0.45363}$$

Average coefficients of friction
for smooth square channels

$$cfrihc6(j,z) = \frac{14.227}{Rehc6_j} \left[1 + 0.046263 \cdot \left(Rehc6_j \cdot \frac{dcell6}{z} \right) \right]^{0.45363}$$

Calculate monolith pressure drop in recuperator with entrance effect:

$$\Delta Phc2_{jcase+1} = 4 \cdot cfrichc2(jcase+1, Lhc) \cdot \frac{Uhc2_{jcase+1}^2}{2} \cdot \rho_{mixhc_{jcase+1}} \cdot \frac{Lhc}{dcell2}$$

$$\Delta Phc4_{jcase+1} = 4 \cdot cfrichc4(jcase+1, Lhc) \cdot \frac{Uhc4_{jcase+1}^2}{2} \cdot \rho_{mixhc_{jcase+1}} \cdot \frac{Lhc}{dcell4}$$

$$\Delta Phc6_{jcase+1} = 4 \cdot cfrichc6(jcase+1, Lhc) \cdot \frac{Uhc6_{jcase+1}^2}{2} \cdot \rho_{mixhc_{jcase+1}} \cdot \frac{Lhc}{dcell6}$$

$$\frac{\Delta Phc2}{Phc} = \begin{bmatrix} 0 \\ 0.0013 \\ 0.0017 \\ 0.002 \\ 0.0024 \\ 0.0041 \end{bmatrix}$$

$$\frac{\Delta Phc4}{Phc} = \begin{bmatrix} 0 \\ 0.0028 \\ 0.0036 \\ 0.0044 \\ 0.0053 \\ 0.0088 \end{bmatrix}$$

$$\frac{\Delta Phc6}{Phc} = \begin{bmatrix} 0 \\ 0.004 \\ 0.0053 \\ 0.0064 \\ 0.0077 \\ 0.0127 \end{bmatrix}$$

$$\Delta Phcmax_P = \begin{bmatrix} 0 \\ 0.003 \\ 0.004 \\ 0.005 \\ 0.006 \\ 0.011 \end{bmatrix}$$

Chose 400 cells per in2
honeycombs via estimated ΔP

Use 400 cells/in2 in honeycomb monolith for calculation of CH4, C7H14, and CO conversions

Find mass transfer rates via Nusselt formulas:

$$Numavghc4c1_{jcase+1} = 2.976 \cdot \left[1 + \left(\frac{7.6 \cdot Lhc}{Rehc4_{jcase+1} \cdot Sc1T(Thc_{jcase+1}) \cdot dcell4} \right)^{\frac{1}{3}} \right]^{\frac{8}{3}}$$

$$Numavghc4c1 = \begin{bmatrix} 0 \\ 2.976 \\ 2.9761 \\ 2.9761 \\ 2.9762 \\ 2.9774 \end{bmatrix}$$

$$Numavghc4co_{jcase+1} = 2.976 \cdot \left[1 + \left(\frac{7.6 \cdot Lhc}{Rehc4_{jcase+1} \cdot ScCoT(Thc_{jcase+1}) \cdot dcell4} \right)^{\frac{1}{3}} \right]^{\frac{8}{3}}$$

$$Numavghc4co = \begin{bmatrix} 0 \\ 2.976 \\ 2.9761 \\ 2.9762 \\ 2.9763 \\ 2.9778 \end{bmatrix}$$

$$\text{Numavghc4c7}_{j\text{case}+1} = 2.976 \cdot \left[1 + \left(\frac{7.6 \cdot \text{Lhc}}{\text{Rehc4}_{j\text{case}+1} \cdot \text{Sc7T}(\text{Thc}_{j\text{case}+1}) \cdot \text{dcell4}} \right)^{\frac{1}{3}} \right]^8$$

$$\text{Numavghc4c7} = \begin{bmatrix} 0 \\ 2.977 \\ 2.9781 \\ 2.9795 \\ 2.9817 \\ 3.0123 \end{bmatrix}$$

Once again the entrance effects within monoliths are generally small

Now determine the maximum possible CH₄, C₇H₁₄, and CO conversions in a 400 cells per in² monolith

$$\text{ych40} := 0.005$$

$$\text{yc7h140} := 0.0005$$

$$\text{yco0} := 0.005$$

$$\text{ych4hc4}_{j\text{case}+1} = \text{ych40} \cdot \exp\left(\frac{-4 \cdot \text{Lhc} \cdot \text{Numavghc4c1}_{j\text{case}+1}}{\text{Rehc4}_{j\text{case}+1} \cdot \text{Sc1T}(\text{Thc}_{j\text{case}+1}) \cdot \text{dcell4}}\right)$$

$$\frac{-4 \cdot \text{Lhc} \cdot \text{Numavghc4c1}_{j\text{case}+1}}{\text{Rehc4}_{j\text{case}+1} \cdot \text{Sc1T}(\text{Thc}_{j\text{case}+1}) \cdot \text{dcell4}}$$

-48.7678
-37.5142
-31.0633
-25.6688
-12.7326

$$\frac{\text{ych4hc4}}{\text{ych40}} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 3.2315 \cdot 10^{-14} \\ 7.1151 \cdot 10^{-12} \\ 2.9532 \cdot 10^{-6} \end{bmatrix}$$

$$\text{ycohc4}_{j\text{case}+1} = \text{yco0} \cdot \exp\left(\frac{-4 \cdot \text{Lhc} \cdot \text{Numavghc4co}_{j\text{case}+1}}{\text{Rehc4}_{j\text{case}+1} \cdot \text{ScCO}(\text{Thc}_{j\text{case}+1}) \cdot \text{dcell4}}\right)$$

$$\frac{\text{ycohc4}}{\text{yco0}} = \begin{bmatrix} 0 \\ 0 \\ 1.4726 \cdot 10^{-15} \\ 5.2301 \cdot 10^{-13} \\ 7.0997 \cdot 10^{-11} \\ 9.1398 \cdot 10^{-6} \end{bmatrix}$$

$$\frac{-4 \cdot \text{Lhc} \cdot \text{Numavghc4co}_{j\text{case}+1}}{\text{Rehc4}_{j\text{case}+1} \cdot \text{ScCO}(\text{Thc}_{j\text{case}+1}) \cdot \text{dcell4}}$$

-44.3966
-34.1518
-28.2792
-23.3684
-11.6029

102230" E9922660

$$yc7h14hc4_{jcase+1} = yc7h140 \cdot \exp\left(\frac{4 \cdot Lhc \cdot Numavghc4c7_{jcase+1}}{Rehc4_{jcase+1} \cdot Sc7T(Thc_{jcase+1}) \cdot dcell4}\right)$$

$$\frac{4 \cdot Lhc \cdot Numavghc4c7_{jcase+1}}{Rehc4_{jcase+1} \cdot Sc7T(Thc_{jcase+1}) \cdot dcell4}$$

· 14.1935
· 10.9219
· 9.0478
· 7.482
· 3.7348

$$\frac{yc7h14hc4}{yc7h140} = \begin{bmatrix} 0 \\ 6.8527 \cdot 10^{-7} \\ 1.8058 \cdot 10^{-5} \\ 0.0001 \\ 0.0006 \\ 0.0239 \end{bmatrix}$$

Only for C7H14 and only in case 5 (maximum power) does the BL transport-only calculated conversion (97.6%) fall below 99.9% with a 400 cells/in2 monolith. With 50 ppm C7H14 in the exhaust in this case, the exit concentration would be 1.2 ppm.

For the final analysis, consider the finite catalytic conversion of C7H14 and CH4 in a monolith: mcase = 5

$$zzcharhc4c7_{jcase+1} = \frac{Rehc4_{jcase+1} \cdot Sc7T(Thc_{jcase+1}) \cdot dcell4}{2}$$

$$\frac{Lhc}{zzcharhc4c7_{mcase}} = 0.6199$$

$$zzcharhc4cl_{jcase+1} = \frac{Rehc4_{jcase+1} \cdot Sc1T(Trecin_{jcase+1}) \cdot dcell4}{2}$$

$$\frac{Lhc}{zzcharhc4cl_{mcase}} = 2.1382$$

$$nz = 400$$

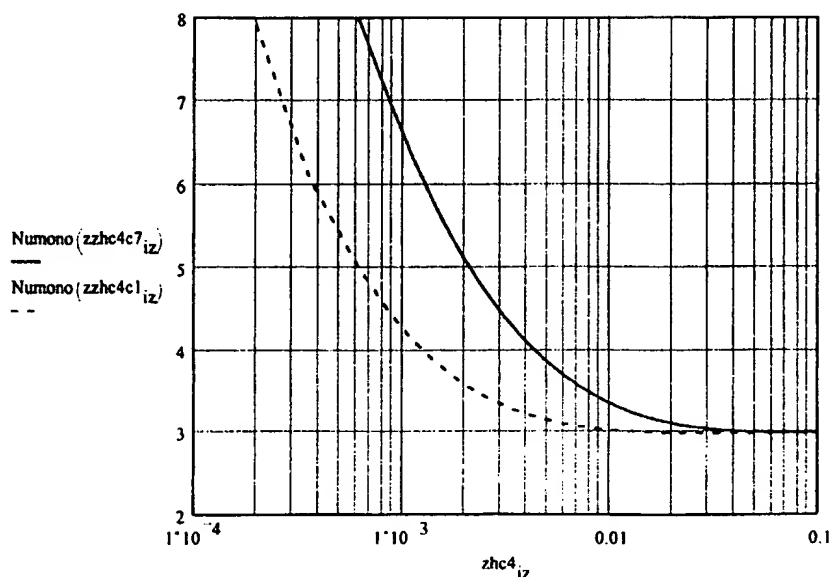
$$Lhc = 10.16 \cdot \text{cm} \quad dcell4 = 0.1168 \cdot \text{cm}$$

$$zhc4_{iz} = iz \cdot \frac{Lhc}{nz} + dwall4$$

$$zzhc4c7_{iz} = \frac{zhc4_{iz}}{zzcharhc4c7_{mcase}}$$

$$zzhc4cl_{iz} = \frac{zhc4_{iz}}{zzcharhc4cl_{mcase}}$$

$$zzcharhc4c7 = \begin{bmatrix} 0 \\ 4.2621 \\ 5.5407 \\ 6.6914 \\ 8.0979 \\ 16.389 \end{bmatrix} \cdot \text{cm}$$



Case specific mcase = 5

$$kgpblhc4c7(T, z) = \frac{Dc7h14T(T) \cdot \text{Numono}\left(\frac{z}{zzcharhc4c7_{mcase}}\right)}{dcell4}$$

$$kgpblhc4c7(Thc_{mcase}, Lhc) = 11.2014 \cdot \text{sec}^{-1} \cdot \text{cm}$$

$$kgpblhc4c1(T, z) = \frac{Dch4T(T) \cdot \text{Numono}\left(\frac{z}{zzcharhc4c1_{mcase}}\right)}{dcell4}$$

$$kgpblhc4c1(Thc_{mcase}, Lhc) = 38.6127 \cdot \text{sec}^{-1} \cdot \text{cm}$$

$$keffhc4c1(T, z) = \frac{1}{\left(\frac{1}{\text{RatekCH4}(kpd(T), T) \cdot Lcat}\right) + \frac{1}{kgpblhc4c1(T, z)}}$$

$$kgpblhc4c1\left(Thc_{mcase}, \frac{Lhc}{2}\right) = 38.615 \cdot \text{sec}^{-1} \cdot \text{cm}$$

$$keffhc4c1\left(Thc_{mcase}, \frac{Lrec}{2}\right) = 1.8533 \cdot \text{sec}^{-1} \cdot \text{cm}$$

$$\text{RatekCH4}(kpd(Thc_{mcase}), Thc_{mcase}) \cdot Lcat = 1.9467 \cdot \text{sec}^{-1} \cdot \text{cm}$$

$$keffhc4c7(T, z) = \frac{1}{\left(\frac{1}{\text{RatekC7H14}(10 \cdot kpd(T), T) \cdot Lcat}\right) + \frac{1}{kgpblhc4c7(T, z)}}$$

$$kgpblhc4c7\left(Thc_{mcase}, \frac{Lhc}{2}\right) = 11.2528 \cdot \text{sec}^{-1} \cdot \text{cm}$$

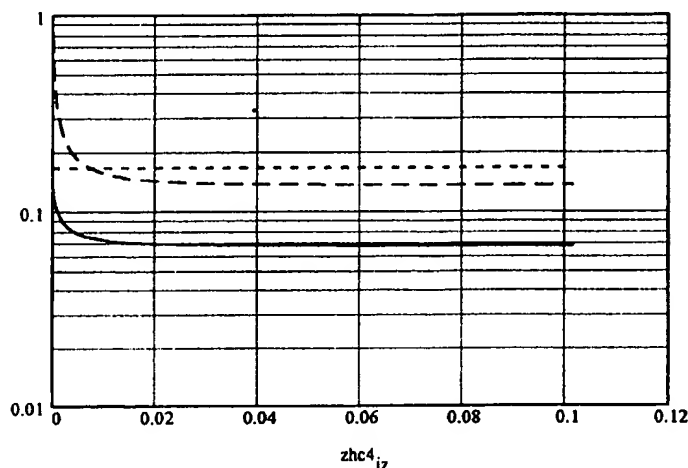
$$keffhc4c7\left(Thc_{mcase}, \frac{Lhc}{2}\right) = 6.7062 \cdot \text{sec}^{-1} \cdot \text{cm}$$

$$\text{RatekC7H14}(10 \cdot kpd(Thc_{mcase}), Thc_{mcase}) \cdot Lcat = 16.5977 \cdot \text{sec}^{-1} \cdot \text{cm}$$

$$\frac{keffhc4c7(Thc_{mcase}, zhc4_{iz})}{\text{RatekC7H14}(10 \cdot kpd(Thc_{mcase}), Thc_{mcase}) \cdot Lcat}$$

$$= \frac{kgpbl6c7(Thc_{mcase}, zhc4_{iz})}{\text{RatekC7H14}(10 \cdot kpd(Thc_{mcase}), Thc_{mcase}) \cdot Lcat}$$

$$= \frac{kgpbl6c7(Thc_{mcase}, zhc4_{iz})}{\text{RatekC7H14}(10 \cdot kpd(Thc_{mcase}), Thc_{mcase}) \cdot Lcat}$$



Determine conversion of fuels with transport-limited finite catalytic combustion rates:

Case specific $m_{case} = 5$

$$yzkhc4c7h14_0 = yz7h140$$

$$yzkhc4ch4_0 = ych40$$

$$Thc = \begin{bmatrix} 0 \\ 1005.3722 \\ 1005.3722 \\ 1005.3722 \\ 1005.3722 \\ 916.4833 \end{bmatrix} \cdot K$$

$$yzkhc4c7h14_{iz+1} = \left(1 - keffhc4c7(Thc_{mcase}, zhc4_{iz}) \cdot \frac{Lhc}{nz} \cdot \frac{4}{dcell4} \cdot \frac{\epsilon_{cell4}}{Uhc4_{mcase}} \right) \cdot yzkhc4c7h14_{iz}$$

$$yzkhc4ch4_{iz+1} = \left(1 - keffhc4c1(Thc_{mcase}, zhc4_{iz}) \cdot \frac{Lhc}{nz} \cdot \frac{4}{dcell4} \cdot \frac{\epsilon_{cell4}}{Uhc4_{mcase}} \right) \cdot yzkhc4ch4_{iz}$$

Case specific

$m_{case} = 5$

$$yzkhc4c7h14_{nz} = 7.281 \cdot 10^{-5}$$

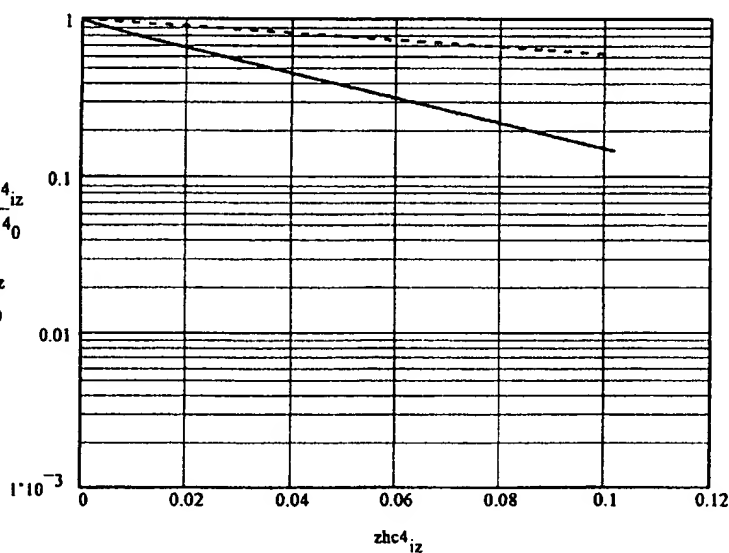
$$yzkhc4c7h14_0 = 0.0005$$

$$yzkhc4ch4_{nz} = 0.003$$

$$yzkhc4ch4_0 = 0.005$$

$$\frac{yzkhc4c7h14_{nz}}{yzkhc4c7h14_0} = 1.456 \cdot 10^{-1}$$

$$\frac{yzkhc4ch4_{nz}}{yzkhc4ch4_0} = 0.5959$$



Case specific $m_{case} = 5$

Conversion of C7H14 under case 5 (full power) is 99.4% [vs. 99.6% via averaged integrated formulas] with about 1-inch entry length. Conversion of CH4 (and also CO) is very high (>99.99%) within about 3.5-inch.

This result shows that the averaged integrated values for CH4, C7H14, and CO conversions are very good approximations and can be used for different values of fuel and CO concentrations.

 Defines transport restricted rate constant given catalyst effective first order rate constant, k_0T , methane or cyclohexane concentration, x , and surface temperature, T

PdO Catalyst Rate Constants

$$\text{Erpd0} := 12800 \cdot K \quad \text{Erpd1} := 4900 \cdot K \quad \text{Erpd3} := 15000 \cdot K$$

Region0 - low T PdO to 625K
 ignores inhibition by H₂O and CO₂

Region1 - Intermediate T
 625K to 909K

Region2 - Flat 909K
 to 1048K decomposition

Region3 -
 Pd metal

$$\text{Apd0} := 2.4 \cdot 10^3 \cdot 200 \cdot \text{gm}^{-1} \cdot \text{sec}^{-1}$$

$$\text{Apd1} := \text{Apd0} \cdot \exp\left(-\frac{\text{Erpd0}}{625 \cdot K} + \frac{\text{Erpd1}}{625 \cdot K}\right)$$

$$\text{Apd2} := \text{Apd1} \cdot \exp\left(-\frac{\text{Erpd1}}{909.1 \cdot K}\right)$$

$$\text{Apd3} := \text{Apd2} \cdot \exp\left(\frac{\text{Erpd3}}{1048.1 \cdot K}\right)$$

Interpolation formula for the four PdO+Pd rate constants

$$\text{kpd}(T) := \left[\text{Apd3}^2 \cdot \exp\left(-\frac{2 \cdot \text{Erpd3}}{T}\right) + \frac{1}{\left(\text{Apd2}^{-2} + \text{Apd1}^{-2} \cdot \exp\left(\frac{2 \cdot \text{Erpd1}}{T}\right) + \text{Apd0}^{-2} \cdot \exp\left(\frac{2 \cdot \text{Erpd0}}{T}\right) \right)} \right]^{0.5}$$

Add expression for Pt(5%)Pd(3.0%) catalyst with C₃H₈ here, use x2 for estimated rate constant with C₇H₁₄:

Rate constant via crushed powder results for C₃H₈

$$\text{ktpdC3}(T) := 6.9 \cdot 10^4 \cdot \exp\left(-\frac{10760 \cdot K}{T}\right) \cdot \text{gm}^{-1} \cdot \text{sec}^{-1}$$

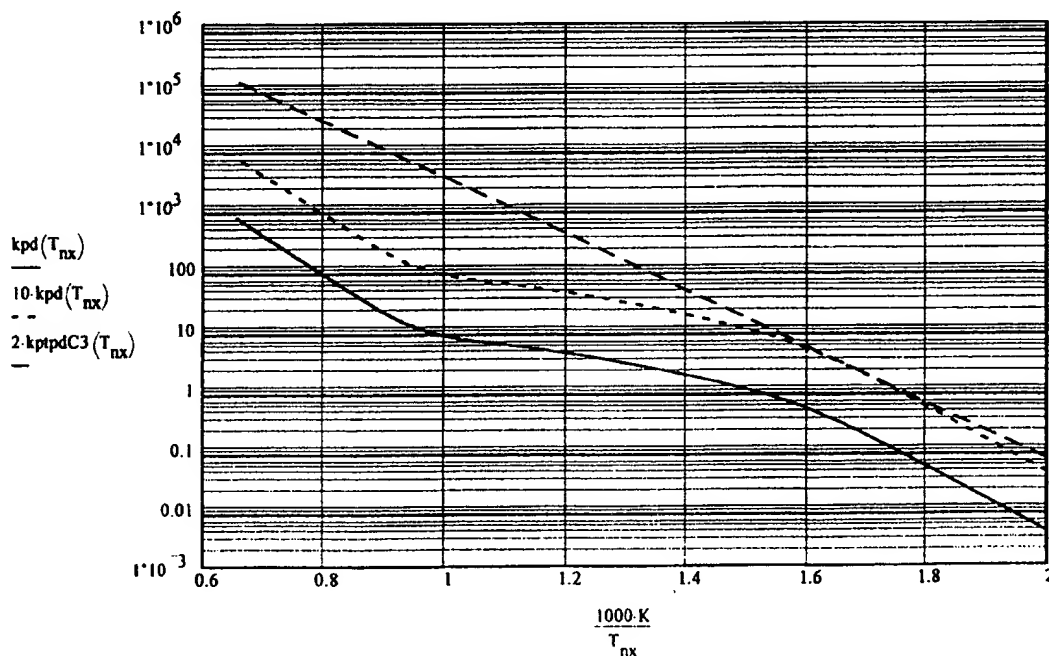
$$10 \cdot \text{kpd}(900 \cdot K) = 49.2392 \cdot \text{kg}^{-1} \cdot \text{sec}^{-1}$$

$$2 \cdot \text{ktpdC3}(900 \cdot K) = 886.4358 \cdot \text{kg}^{-1} \cdot \text{sec}^{-1}$$

$$\text{nx} := 0, 1 \dots 41$$

$$T_{\text{nx}} := 500 \cdot K + \text{nx} \cdot 25 \cdot K$$

CATALYTIC RATE CONSTANT vs TEMPERATURE
 (mol/atmCH_x/s/gcat)

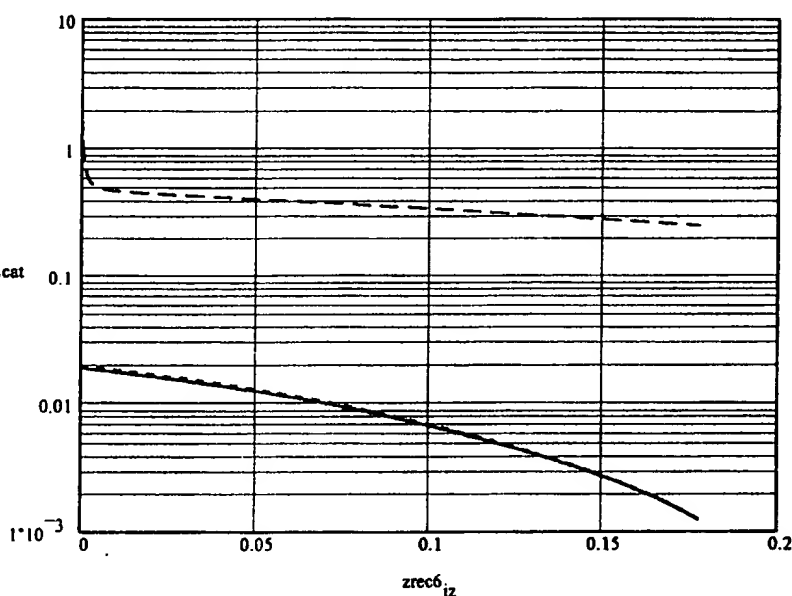


$$\text{keffrec6c1}(T, z) = \frac{1}{\left(\frac{1}{\text{RatekCH4}(\text{kpd}(T), T) \cdot \text{Lcat}} \right) + \frac{1}{\text{kgpb16c1}(T, z)}} \quad \text{kgpb16c1}\left(\text{Tavg}_{\text{ncase}}, \frac{\text{Lrec}}{2}\right) = 35.3023 \cdot \text{sec}^{-1} \cdot \text{cm}$$

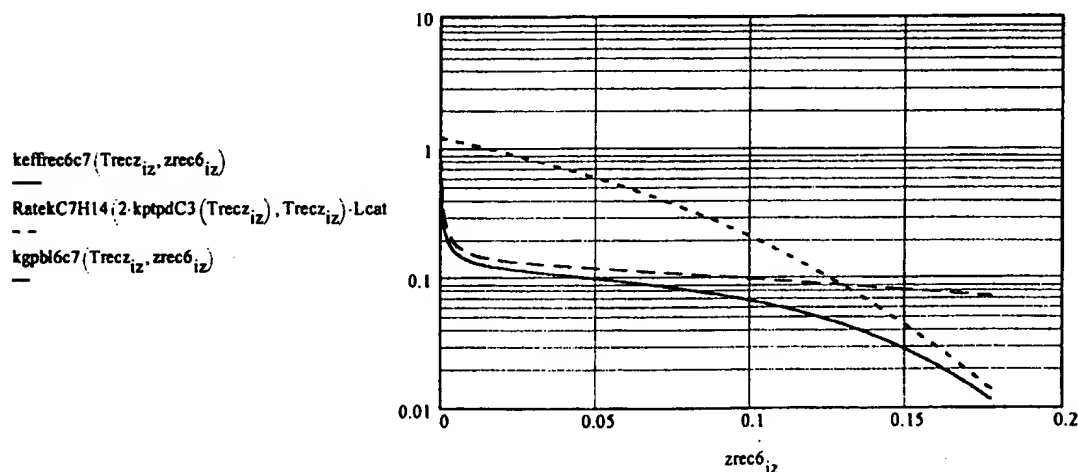
$$\text{keffrec6c1}\left(\text{Tavg}_{\text{ncase}}, \frac{\text{Lrec}}{2}\right) = 0.7922 \cdot \text{sec}^{-1} \cdot \text{cm} \quad \text{RatekCH4}(\text{kpd}(\text{Tavg}_{\text{ncase}}), \text{Tavg}_{\text{ncase}}) \cdot \text{Lcat} = 0.8104 \cdot \text{sec}^{-1} \cdot \text{cm}$$

$$\text{keffrec6c7}(T, z) = \frac{1}{\left(\frac{1}{\text{RatekC7H14}(2 \cdot \text{ktpdC3}(T), T) \cdot \text{Lcat}} \right) + \frac{1}{\text{kgpb16c7}(T, z)}} \quad \text{kgpb16c7}\left(\text{Tavg}_{\text{ncase}}, \frac{\text{Lrec}}{2}\right) = 10.1756 \cdot \text{sec}^{-1} \cdot \text{cm}$$

$$\text{keffrec6c7}\left(\text{Tavg}_{\text{ncase}}, \frac{\text{Lrec}}{2}\right) = 7.4067 \cdot \text{sec}^{-1} \cdot \text{cm} \quad \text{RatekC7H14}(2 \cdot \text{ktpdC3}(\text{Tavg}_{\text{ncase}}), \text{Tavg}_{\text{ncase}}) \cdot \text{Lcat} = 27.2196 \cdot \text{sec}^{-1} \cdot \text{cm}$$



Case specific $\text{ncase} = 5$



002280-099EE660

$$\text{Trecz}_{iz} \quad \text{Trecin}_{ncase} \quad \text{Trecin}_{ncase} \quad \text{Trecout}_{ncase} \quad \text{Trecout}_{ncase} \quad \text{Trecz}_{iz}$$

$$\text{Trecz}_{nz} = 630.3722 \cdot K \quad \text{Trecout}_{ncase} = 630.3722 \cdot K$$

$$\mathbf{yzkc7h14}_0 = \mathbf{yc7h140} \qquad \mathbf{yzkch4}_0 := \mathbf{ych40}$$

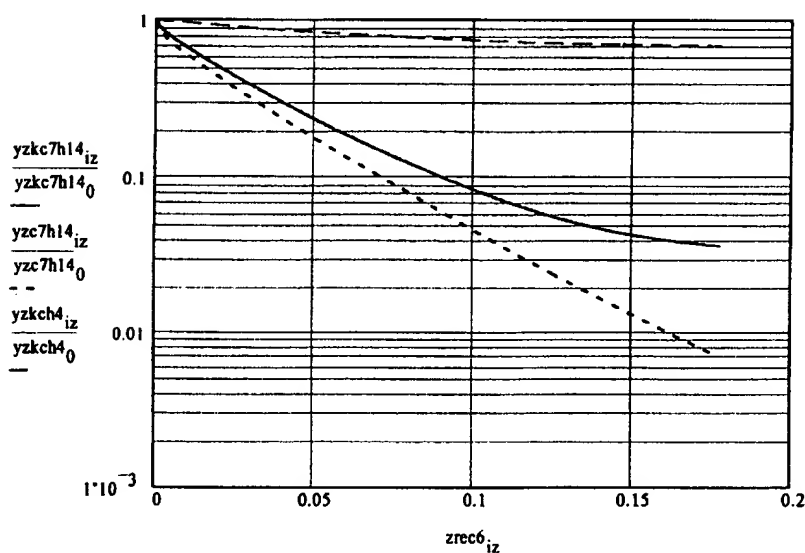
$$yzkc7h14_{iz+1} = \left(1 - keffrec6c7(Trecz_{iz}, zrec6_{iz}) \cdot \frac{Lrec}{nz} \cdot 1.1 \cdot \frac{4}{dcell6} \cdot \frac{\&cell6}{Urec_{ncase}} \cdot \frac{Trecin_5}{Trecz_{iz}}\right) \cdot yzkc7h14_{iz}$$

Case specific

$$yzkch4_{iz+1} = \left(1 - keffrec6cl(Trecz_{iz}, zrec6_{iz}) \cdot \frac{Lrec}{nz} \cdot 1.1 \cdot \frac{4}{dccl6} \cdot \frac{scell6}{Urec_{ncase}} \cdot \frac{Trecin_5}{Trecz_{iz}} \right) \cdot yzkch4_{iz}$$

Case specific

$$\begin{array}{llll} \text{yzkc7h14}_{\text{nz}} = 1.802 \cdot 10^{-5} & \text{yzkc7h14}_0 = 0.0005 & \frac{\text{yzkc7h14}_{\text{nz}}}{\text{yzkc7h14}_0} = 3.603 \cdot 10^{-2} & \frac{\text{yzkch4}_{\text{nz}}}{\text{yzkch4}_0} = 0.6838 \\ \text{yzkch4}_{\text{nz}} = 0.0034 & \text{yzkch4}_0 = 0.005 & & \end{array}$$



Conversion of C7H14 under case 5 (full power) is 97.4% with estimated catalytic rates and transport limitations [vs. 99.6% for the maximum BL transport-limited conversion]. Conversion of CH4 is very poor (32%). CO conversion is probably very high given higher catalytic and transport rates than with C7H14.

This result shows that the specific rates of catalytic oxidation of all added components needs to be measured as applied to a recuperator. The use of a recuperator for emission control would appear to be greatly enhanced with higher exhaust (recuperator) temperatures.

In the following section, the conversion of C_7H_{14} , CH_4 and CO is considered for various honeycomb monoliths

$$Thc_{jcase+1} = Trecin_{jcase+1} \quad \rho_{mixhc_{jcase+1}} = \rho_{mixrec}(Trecin_{jcase+1})$$

$$Ghc2_{jcase+1} = \frac{mf_{jcase+1}}{Shc \cdot \epsilon_{cell2}} \quad Ghc4_{jcase+1} = \frac{mf_{jcase+1}}{Shc \cdot \epsilon_{cell4}} \quad Ghc6_{jcase+1} = \frac{mf_{jcase+1}}{Shc \cdot \epsilon_{cell6}}$$

$$Uhc2 = \begin{bmatrix} 0 \\ 3.058 \\ 3.9753 \\ 4.801 \\ 5.8101 \\ 10.0353 \end{bmatrix} \cdot m \cdot sec^{-1}$$

$$Uhc4 = \begin{bmatrix} 0 \\ 3.2157 \\ 4.1804 \\ 5.0487 \\ 6.1098 \\ 10.553 \end{bmatrix} \cdot m \cdot sec^{-1}$$

$$Uhc6 = \begin{bmatrix} 0 \\ 3.1706 \\ 4.1218 \\ 4.9779 \\ 6.0242 \\ 10.4051 \end{bmatrix} \cdot m \cdot sec^{-1}$$

Evaluate Reynolds numbers for use in calculating the momentum, heat, and mass transfer functions:

$$Rehc2_{jcase+1} = \frac{Ghc2_{jcase+1} \cdot d_{cell2}}{\mu_{mixT}(Thc_{jcase+1})}$$

$$Rehc4_{jcase+1} = \frac{Ghc4_{jcase+1} \cdot d_{cell4}}{\mu_{mixT}(Thc_{jcase+1})}$$

$$Rehc6_{jcase+1} = \frac{Ghc6_{jcase+1} \cdot d_{cell6}}{\mu_{mixT}(Thc_{jcase+1})}$$

$$Rehc2 = \begin{bmatrix} 0 \\ 43.776 \\ 56.9088 \\ 68.7283 \\ 83.1744 \\ 167.4548 \end{bmatrix}$$

$$Rehc4 = \begin{bmatrix} 0 \\ 31.7427 \\ 41.2655 \\ 49.836 \\ 60.3111 \\ 121.4242 \end{bmatrix}$$

$$Rehc6 = \begin{bmatrix} 0 \\ 25.7355 \\ 33.4562 \\ 40.4048 \\ 48.8975 \\ 98.4453 \end{bmatrix}$$

$$cfrichc2(j,z) = \frac{14.227}{Rehc2_j} \left[1 + 0.046263 \cdot \left(Rehc2_j \cdot \frac{d_{cell2}}{z} \right)^{0.45363} \right]$$

$$cfrichc4(j,z) = \frac{14.227}{Rehc4_j} \left[1 + 0.046263 \cdot \left(Rehc4_j \cdot \frac{d_{cell4}}{z} \right)^{0.45363} \right]$$

Average coefficients of friction
for smooth square channels

$$cfrichc6(j,z) = \frac{14.227}{Rehc6_j} \left[1 + 0.046263 \cdot \left(Rehc6_j \cdot \frac{d_{cell6}}{z} \right)^{0.45363} \right]$$

Calculate monolith pressure drop in recuperator with entrance effect:

$$\Delta P_{hc2, jcase+1} = 4 \cdot cfrichc2(jcase+1, Lhc) \cdot \frac{(U_{hc2, jcase+1})^2}{2} \cdot \rho_{mixhc, jcase+1} \cdot \frac{Lhc}{d_{cell2}}$$

$$\Delta P_{hc4, jcase+1} = 4 \cdot cfrichc4(jcase+1, Lhc) \cdot \frac{(U_{hc4, jcase+1})^2}{2} \cdot \rho_{mixhc, jcase+1} \cdot \frac{Lhc}{d_{cell4}}$$

$$\Delta P_{hc6, jcase+1} = 4 \cdot cfrichc6(jcase+1, Lhc) \cdot \frac{(U_{hc6, jcase+1})^2}{2} \cdot \rho_{mixhc, jcase+1} \cdot \frac{Lhc}{d_{cell6}}$$

$$\frac{\Delta P_{hc2}}{Phc} = \begin{bmatrix} 0 \\ 0.0013 \\ 0.0017 \\ 0.002 \\ 0.0024 \\ 0.0041 \end{bmatrix} \quad \frac{\Delta P_{hc4}}{Phc} = \begin{bmatrix} 0 \\ 0.0028 \\ 0.0036 \\ 0.0044 \\ 0.0053 \\ 0.0088 \end{bmatrix} \quad \frac{\Delta P_{hc6}}{Phc} = \begin{bmatrix} 0 \\ 0.004 \\ 0.0053 \\ 0.0064 \\ 0.0077 \\ 0.0127 \end{bmatrix} \quad \frac{3.5}{4} \frac{\Delta P_{hc6}}{Phc} = \begin{bmatrix} 0 \\ 0.0035 \\ 0.0046 \\ 0.0056 \\ 0.0068 \\ 0.0111 \end{bmatrix} \quad \Delta P_{hcmax_P} = \begin{bmatrix} 0 \\ 0.003 \\ 0.004 \\ 0.005 \\ 0.006 \\ 0.011 \end{bmatrix}$$

Chose 600 cells per in² honeycombs but
reduce length to 3.5in via estimated ΔP

Lhc := 3.5-in

Use 600 cells/in² in honeycomb monolith for calculation of CH₄, C₇H₁₄, and CO conversions

Find mass transfer rates via Nusselt formulas:

$$Numavghc6cl_{jcase+1} = 2.976 \cdot \left[1 + \left(\frac{7.6 \cdot Lhc}{Re_{hc6, jcase+1} \cdot Sc_{lT}(Thc_{jcase+1}) \cdot d_{cell6}} \right)^{\frac{1}{3}} \right]^{\frac{1}{8}}$$

$$Numavghc6cl = \begin{bmatrix} 0 \\ 2.976 \\ 2.976 \\ 2.9761 \\ 2.9761 \\ 2.9767 \end{bmatrix}$$

$$Numavghc6co_{jcase+1} = 2.976 \cdot \left[1 + \left(\frac{7.6 \cdot Lhc}{Re_{hc6, jcase+1} \cdot Sc_{coT}(Thc_{jcase+1}) \cdot d_{cell6}} \right)^{\frac{1}{3}} \right]^{\frac{1}{8}}$$

$$Numavghc6co = \begin{bmatrix} 0 \\ 2.976 \\ 2.976 \\ 2.9761 \\ 2.9761 \\ 2.9769 \end{bmatrix}$$

$$\text{Numavghc6c7}_{j\text{case}+1} = 2.976 \cdot \left[1 + \left(\frac{7.6 \cdot \text{Lhc}}{\text{Rehc6}_{j\text{case}+1} \cdot \text{Sc7T}(\text{Thc}_{j\text{case}+1}) \cdot \text{dcell6}} \right)^{\frac{1}{3}} \right]^{\frac{8}{3}}$$

$$\text{Numavghc6c7} = \begin{bmatrix} 0 \\ 2.9765 \\ 2.977 \\ 2.9777 \\ 2.9788 \\ 2.994 \end{bmatrix}$$

Once again the entrance effects within monoliths are generally small

Now determine the maximum possible CH₄, C₇H₁₄, and CO conversions in a 600 cells per in² monolith

$$\text{ych40} = 0.005$$

$$\text{yc7h140} = 0.0005$$

$$\text{yc0} = 0.005$$

$$\text{ych4hc6}_{j\text{case}+1} = \text{ych40} \cdot \exp \left(\frac{-4 \cdot \text{Lhc} \cdot \text{Numavghc6c1}_{j\text{case}+1}}{\text{Rehc6}_{j\text{case}+1} \cdot \text{Sc1T}(\text{Thc}_{j\text{case}+1}) \cdot \text{dcell6}} \right)$$

$$\frac{-4 \cdot \text{Lhc} \cdot \text{Numavghc6c1}_{j\text{case}+1}}{\text{Rehc6}_{j\text{case}+1} \cdot \text{Sc1T}(\text{Thc}_{j\text{case}+1}) \cdot \text{dcell6}}$$

-64.0074
-49.2367
-40.7696
-33.689
-16.7076

$$\frac{\text{ych4hc6}}{\text{ych40}} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 2.339 \cdot 10^{-15} \\ 5.5463 \cdot 10^{-8} \end{bmatrix}$$

$$\text{ycoh6}_{j\text{case}+1} = \text{yc0} \cdot \exp \left(\frac{-4 \cdot \text{Lhc} \cdot \text{Numavghc6co}_{j\text{case}+1}}{\text{Rehc6}_{j\text{case}+1} \cdot \text{Sc0T}(\text{Thc}_{j\text{case}+1}) \cdot \text{dcell6}} \right)$$

$$\frac{-4 \cdot \text{Lhc} \cdot \text{Numavghc6co}_{j\text{case}+1}}{\text{Rehc6}_{j\text{case}+1} \cdot \text{Sc0T}(\text{Thc}_{j\text{case}+1}) \cdot \text{dcell6}}$$

-58.27
-44.8234
-37.1153
-30.6695
-15.2241

$$\frac{\text{ycoh6}}{\text{yc0}} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 4.7906 \cdot 10^{-14} \\ 2.445 \cdot 10^{-7} \end{bmatrix}$$

T02280" E99E660

$$yc7h14hc6_{jcase+1} = yc7h140 \cdot \exp\left(\frac{-3.5 \cdot Lhc \cdot Numavghc6c7_{jcase+1}}{Rehc6_{jcase+1} \cdot Sc7T(Thc_{jcase+1}) \cdot dcell6}\right)$$

$$\frac{yc7h14hc6}{yc7h140} = \frac{-3.5 \cdot Lhc \cdot Numavghc6c7_{jcase+1}}{Rehc6_{jcase+1} \cdot Sc7T(Thc_{jcase+1}) \cdot dcell6}$$

$$\frac{yc7h14hc6}{yc7h140} = \begin{bmatrix} 0 \\ 8.3588 \cdot 10^{-8} \\ 3.5856 \cdot 10^{-6} \\ 3.0905 \cdot 10^{-5} \\ 0.0002 \\ 0.0141 \end{bmatrix}$$

$$\begin{bmatrix} -16.2974 \\ -12.5386 \\ -10.3846 \\ -8.5841 \\ -4.2631 \end{bmatrix}$$

Only for C7H14 and only in case 5 (maximum power) does the BL transport-only calculated conversion (98.6%) fall below 99.9% with a 600 cells/in² monolith. With 50 ppm C7H14 in the exhaust in this case, the exit concentration would be 0.7 ppm.

For the final analysis, consider the finite catalytic conversion of C7H14 and CH4 in a monolith: mcase := 5

$$zzcharhc6c7_{jcase+1} := \frac{Rehc6_{jcase+1} \cdot Sc7T(Thc_{jcase+1}) \cdot dcell6}{2}$$

$$\frac{Lhc}{zzcharhc6c7_{mcase}} = 0.8137$$

$$zzcharhc6c1_{jcase+1} := \frac{Rehc6_{jcase+1} \cdot Sc1T(Trecin_{jcase+1}) \cdot dcell6}{2}$$

$$\frac{Lhc}{zzcharhc6c1_{mcase}} = 2.8064$$

$$nz = 400$$

$$Lhc = 8.89 \cdot \text{cm}$$

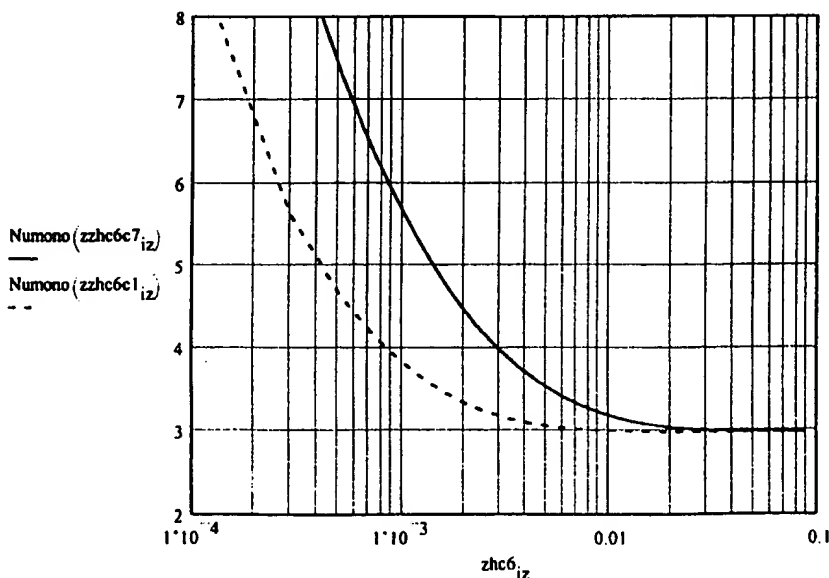
$$dcell6 = 0.0961 \cdot \text{cm}$$

$$zhc6_{iz} := iz \cdot \frac{Lhc}{nz} + dwall6$$

$$zzhc6c7_{iz} := \frac{zhc6_{iz}}{zzcharhc6c7_{mcase}}$$

$$zzhc6c1_{iz} := \frac{zhc6_{iz}}{zzcharhc6c1_{mcase}}$$

$$zzcharhc6c7 = \begin{bmatrix} 0 \\ 2.8414 \\ 3.6938 \\ 4.461 \\ 5.3986 \\ 10.926 \end{bmatrix} \cdot \text{cm}$$



$$kgpblhc6c7(T, z) := \frac{Dc7h14T(T) \cdot \text{Numono}\left(\frac{z}{zzcharhc6c7_{mcase}}\right)}{dcell6}$$

Case specific mcase = 5

$$kgpblhc6c7(Thc_{mcase}, Lhc) = 13.6172 \cdot \text{sec}^{-1} \cdot \text{cm}$$

$$kgpblhc6c1(T, z) := \frac{Dch4T(T) \cdot \text{Numono}\left(\frac{z}{zzcharhc6c1_{mcase}}\right)}{dcell6}$$

$$kgpblhc6c1(Thc_{mcase}, Lhc) = 46.9581 \cdot \text{sec}^{-1} \cdot \text{cm}$$

$$keffhc6c1(T, z) := \frac{1}{\left(\frac{1}{\text{RatekCH4}(kpd(T), T) \cdot Lcat}\right) + \frac{1}{kgpblhc6c1(T, z)}}$$

$$kgpblhc6c1\left(Thc_{mcase}, \frac{Lhc}{2}\right) = 46.9589 \cdot \text{sec}^{-1} \cdot \text{cm}$$

$$keffhc6c1\left(Thc_{mcase}, \frac{Lrec}{2}\right) = 1.8693 \cdot \text{sec}^{-1} \cdot \text{cm}$$

$$\text{RatekCH4}(kpd(Thc_{mcase}), Thc_{mcase}) \cdot Lcat = 1.9467 \cdot \text{sec}^{-1} \cdot \text{cm}$$

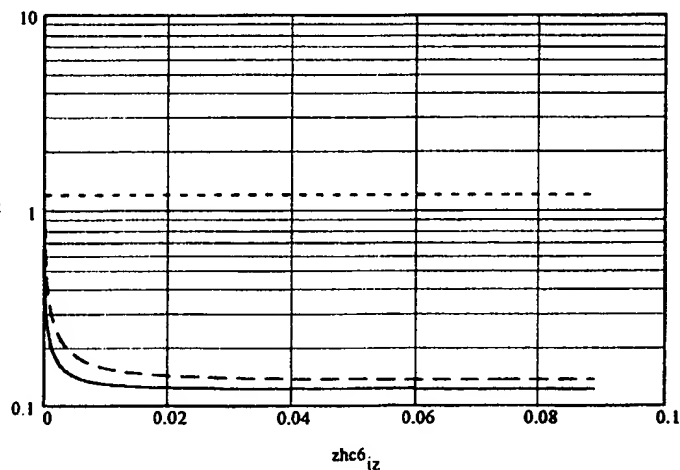
$$keffhc6c7(T, z) := \frac{1}{\left(\frac{1}{\text{RatekC7H14}(2 \cdot ktpdC3(T), T) \cdot Lcat}\right) + \frac{1}{kgpblhc6c7(T, z)}}$$

$$kgpblhc6c7\left(Thc_{mcase}, \frac{Lhc}{2}\right) = 13.6468 \cdot \text{sec}^{-1} \cdot \text{cm}$$

$$keffhc6c7\left(Thc_{mcase}, \frac{Lhc}{2}\right) = 12.2537 \cdot \text{sec}^{-1} \cdot \text{cm}$$

$$\text{RatekC7H14}(2 \cdot ktpdC3(Thc_{mcase}), Thc_{mcase}) \cdot Lcat = 120.0371 \cdot \text{sec}^{-1} \cdot \text{cm}$$

$$\frac{keffhc6c7(Thc_{mcase}, zhc6_{iz})}{\text{RatekC7H14}(2 \cdot ktpdC3(Thc_{mcase}), Thc_{mcase}) \cdot Lcat} - \frac{kgpblhc6c7(Thc_{mcase}, zhc6_{iz})}{1}$$



Determine conversion of fuels with transport-limited finite catalytic combustion rates:

Case specific

$$mcase = 5$$

$$yzkhc6c7h14_0 = yz7h140$$

$$yzkhc6ch4_0 = ych40$$

$$Thc = \begin{bmatrix} 0 \\ 1005.3722 \\ 1005.3722 \\ 1005.3722 \\ 1005.3722 \\ 916.4833 \end{bmatrix} \cdot K$$

$$yzkhc6c7h14_{iz+1} = \left(1 - keffhc6c7(Thc_{mcase}, zhc6_{iz}) \cdot \frac{Lhc}{nz} \cdot \frac{4}{dcell6} \cdot \frac{\epsilon_{cell6}}{Uhc6_{mcase}} \right) \cdot yzkhc6c7h14_{iz}$$

$$yzkhc6ch4_{iz+1} = \left(1 - keffhc6c1(Thc_{mcase}, zhc6_{iz}) \cdot \frac{Lhc}{nz} \cdot \frac{4}{dcell6} \cdot \frac{\epsilon_{cell4}}{Uhc6_{mcase}} \right) \cdot yzkhc6ch4_{iz}$$

Case specific

$$mcase = 5$$

$$yzkhc6c7h14_{nz} = 9.964 \cdot 10^{-6}$$

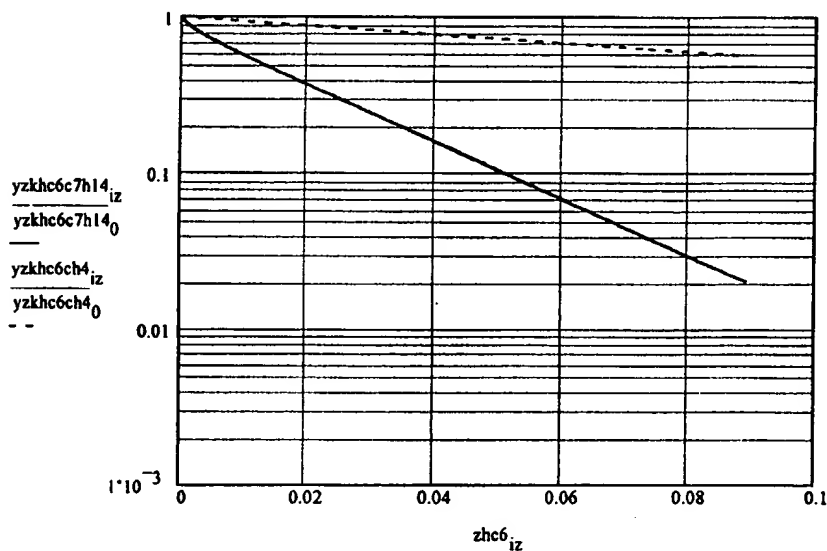
$$yzkhc6c7h14_0 = 0.0005$$

$$yzkhc6ch4_{nz} = 0.0028$$

$$yzkhc6ch4_0 = 0.005$$

$$\frac{yzkhc6c7h14_{nz}}{yzkhc6c7h14_0} = 1.993 \cdot 10^{-2}$$

$$\frac{yzkhc6ch4_{nz}}{yzkhc6ch4_0} = 0.5693$$



Case specific $mcase = 5$

Conversion of C7H14 under case 5 (full power) with 600 cells/in² x 3.5-in length and extrapolated catalytic rates (via C3H8 at 400C) is 98.0% [vs. 99.6% via averaged integrated formulas, 99.3% with temperature dependent transport, and 98.6% with 400 cells/in² and 4-in length. Conversion of CH4 is limited by slow kinetics and CO is expected to be very high (>99.99%).

 Gas Properties and Constants

$\text{cm} \equiv 0.01 \cdot \text{m}$ $\text{J} \equiv \text{kg} \cdot \text{m}^2 \cdot \text{sec}^{-2}$ $\text{W} \equiv \text{J} \cdot \text{sec}^{-1}$ $\text{Pref} \equiv 1 \cdot \text{atm}$
 $\text{N} \equiv \text{kg} \cdot \text{m} \cdot \text{sec}^{-2}$ $\text{Pa} \equiv \text{N} \cdot \text{m}^{-2}$ $\text{atm} \equiv 101300 \cdot \text{Pa}$ $\mu\text{m} \equiv 0.000001 \cdot \text{m}$
 $R \equiv 8.3143 \cdot \frac{\text{J}}{\text{K}}$ $R_c \equiv 8.3143 \cdot \text{J} \cdot \text{mole}^{-1} \cdot \text{K}^{-1}$

n	Gas	MolWt	$\sigma(\text{LJ})$	$\epsilon(\text{LJ})$
1	CH4	$\text{MW}_0 \equiv 16.044 \cdot \text{gm}$	$\sigma_0 \equiv 3.785 \cdot 10^{-10} \cdot \text{m}$	$\epsilon_0 \equiv 148.6 \cdot \text{K}$
2	O2	$\text{MW}_1 \equiv 31.999 \cdot \text{gm}$	$\sigma_1 \equiv 3.464 \cdot 10^{-10} \cdot \text{m}$	$\epsilon_1 \equiv 106.7 \cdot \text{K}$
3	N2	$\text{MW}_2 \equiv 28.018 \cdot \text{gm}$	$\sigma_2 \equiv 3.798 \cdot 10^{-10} \cdot \text{m}$	$\epsilon_2 \equiv 71.4 \cdot \text{K}$
4	CO2	$\text{MW}_3 \equiv 44.010 \cdot \text{gm}$	$\sigma_3 \equiv 3.941 \cdot 10^{-10} \cdot \text{m}$	$\epsilon_3 \equiv 195.2 \cdot \text{K}$
5	H2O	$\text{MW}_4 \equiv 18.015 \cdot \text{gm}$	$\sigma_4 \equiv 2.641 \cdot 10^{-10} \cdot \text{m}$	$\epsilon_4 \equiv 809.1 \cdot \text{K}$

Define transport integrals:

Constants:

$\sigma\mu a_0 \equiv 1.16145$	$\sigma\mu b_0 \equiv 0.14874$	$\sigma\text{Da}_0 \equiv 1.06036$	$\sigma\text{Db}_0 \equiv 0.1561$
$\sigma\mu a_1 \equiv 0.52487$	$\sigma\mu b_1 \equiv 0.7732$	$\sigma\text{Da}_1 \equiv 0.193$	$\sigma\text{Db}_1 \equiv 0.47635$
$\sigma\mu a_2 \equiv 2.16178$	$\sigma\mu b_2 \equiv 2.43787$	$\sigma\text{Da}_2 \equiv 1.03587$	$\sigma\text{Db}_2 \equiv 1.52996$
		$\sigma\text{Da}_3 \equiv 1.76474$	$\sigma\text{Db}_3 \equiv 3.89411$

Functions:

$$\Omega\mu(T) \equiv \sigma\mu a_0 \cdot \exp[-(\sigma\mu b_0 \cdot \ln(T))] + \sum_{i\mu=1}^2 \sigma\mu a_{i\mu} \cdot \exp(-\sigma\mu b_{i\mu} \cdot T) \quad \Omega\mu(3) = 1.0394$$

$$\Omega D(T) \equiv \sigma\text{Da}_0 \cdot \exp[-(\sigma\text{Db}_0 \cdot \ln(T))] + \sum_{iD=1}^3 \sigma\text{Da}_{iD} \cdot \exp(-\sigma\text{Db}_{iD} \cdot T) \quad \Omega D(3) = 0.95002$$

B5
B4

Set Inlet Conditions:

$$P := 1.0\text{-atm} \quad y_{ch40} := 0.035$$

Define gas composition w/r methane using moist (3%) air:

$$y(x) := \begin{bmatrix} x \\ (1 - y_{ch40}) \cdot 0.2 - 2 \cdot y_{ch40} + 2 \cdot x \\ (1 - y_{ch40}) \cdot 0.77 \\ y_{ch40} - x \\ (1 - y_{ch40}) \cdot 0.03 + 2 \cdot y_{ch40} - 2 \cdot x \end{bmatrix} \quad y(0.02) = \begin{bmatrix} 0.02 \\ 0.163 \\ 0.743 \\ 0.015 \\ 0.059 \end{bmatrix}$$

Define viscosity function

$$\mu(T) = \begin{bmatrix} \frac{2.6693 \cdot 10^{-26} \cdot (MW_0 \cdot T)^{0.5}}{(\sigma_0)^2 \cdot \Omega \mu \left(\frac{T}{\epsilon_0} \right)} \cdot \frac{10^5 \cdot \text{cm}}{\text{sec}} \cdot \left(\frac{\text{gm}}{\text{K}} \right)^{0.5} \\ \frac{(MW_1 \cdot T)^{0.5}}{(\sigma_1)^2 \cdot \Omega \mu \left(\frac{T}{\epsilon_1} \right)} \cdot \left[2.6693 \cdot 10^{-26} \cdot \left(\frac{10^5 \cdot \text{cm}}{\text{sec}} \right) \cdot \left(\frac{\text{gm}}{\text{K}} \right)^{0.5} \right] \\ \frac{(MW_2 \cdot T)^{0.5}}{(\sigma_2)^2 \cdot \Omega \mu \left(\frac{T}{\epsilon_2} \right)} \cdot \left[2.6693 \cdot 10^{-26} \cdot \left(\frac{10^5 \cdot \text{cm}}{\text{sec}} \right) \cdot \left(\frac{\text{gm}}{\text{K}} \right)^{0.5} \right] \\ \frac{(MW_3 \cdot T)^{0.5}}{(\sigma_3)^2 \cdot \Omega \mu \left(\frac{T}{\epsilon_3} \right)} \cdot \left[2.6693 \cdot 10^{-26} \cdot \left(\frac{10^5 \cdot \text{cm}}{\text{sec}} \right) \cdot \left(\frac{\text{gm}}{\text{K}} \right)^{0.5} \right] \\ \frac{1.116 \cdot (MW_4 \cdot T)^{0.5}}{(3.115 \cdot 10^{-8} \cdot \text{cm})^2 \cdot \Omega \mu \left(\frac{T}{514 \cdot \text{K}} \right)} \cdot \left[2.6693 \cdot 10^{-26} \cdot \left(\frac{10^5 \cdot \text{cm}}{\text{sec}} \right) \cdot \left(\frac{\text{gm}}{\text{K}} \right)^{0.5} \right] \end{bmatrix} \quad \mu(300 \cdot \text{K}) = \begin{bmatrix} 1.103 \cdot 10^{-5} \\ 2.06 \cdot 10^{-5} \\ 1.77 \cdot 10^{-5} \\ 1.519 \cdot 10^{-5} \\ 1.068 \cdot 10^{-5} \end{bmatrix} \cdot \text{kg} \cdot \text{m}^{-1} \cdot \text{sec}^{-1}$$

T02280.E99EE660

$$\mu_{\text{mix}}(x, T) := \sum_{n=0}^4 \frac{y(x)_n \cdot (\mu(T))_n}{\sum_{m=0}^4 y(x)_m \cdot \frac{\left[1 + \left(\frac{\mu(T)_n}{\mu(T)_m} \right)^{0.5} \cdot \left(\frac{MW_m}{MW_n} \right)^{0.25} \right]^2}{\left[8 \cdot \left(1 + \frac{MW_n}{MW_m} \right) \right]^{0.5}}}$$

$$y(0.02) = \begin{bmatrix} 0.02 \\ 0.163 \\ 0.743 \\ 0.015 \\ 0.059 \end{bmatrix}$$

$$\mu_{\text{mix}}(0.02, 300 \cdot K) = 1.759 \cdot 10^{-5} \cdot \text{kg} \cdot \text{m}^{-1} \cdot \text{sec}^{-1}$$

Define thermal conductivity functions

igas := 0, 1 .. 4

$$a\lambda = \begin{bmatrix} -1.869 \\ -0.3273 \\ 0.3919 \\ -7.215 \\ 7.341 \end{bmatrix} \quad b\lambda = \begin{bmatrix} 0.08727 \\ 0.09966 \\ 0.09816 \\ 0.08015 \\ -0.01013 \end{bmatrix} \quad c\lambda = \begin{bmatrix} 1.179 \cdot 10^{-4} \\ - (3.743 \cdot 10^{-5}) \\ - (5.067 \cdot 10^{-5}) \\ 5.477 \cdot 10^{-6} \\ 1.801 \cdot 10^{-4} \end{bmatrix} \quad d\lambda = \begin{bmatrix} - (3.614 \cdot 10^{-8}) \\ 9.732 \cdot 10^{-9} \\ 1.504 \cdot 10^{-8} \\ - (1.053 \cdot 10^{-8}) \\ - (9.1 \cdot 10^{-8}) \end{bmatrix}$$

CH4
O2
N2
CO2
H2O

$$\lambda(i, T) := \left[a\lambda_i + b\lambda_i \cdot \frac{T}{K} + c\lambda_i \cdot \left(\frac{T}{K} \right)^2 + d\lambda_i \cdot \left(\frac{T}{K} \right)^3 \right] \cdot 0.00001 \cdot \frac{W}{\text{cm} \cdot K} \quad W/\text{cm} \cdot K$$

$$\lambda_{\text{mix}}(x, T) := \sum_{i=0}^4 \frac{y(x)_i \cdot \lambda(i, T)}{\sum_{j=0}^4 y(x)_j \cdot \frac{\left[1 + \left(\frac{\mu(T)_i}{\mu(T)_j} \right)^{0.5} \cdot \left(\frac{MW_j}{MW_i} \right)^{0.25} \right]^2}{\left[8 \cdot \left(1 + \frac{MW_i}{MW_j} \right) \right]^{0.5}}}$$

$\lambda(\text{igas}, 1000 \cdot K)$

0.16716 · kg · m · sec ⁻³ · K ⁻¹
0.07163 · kg · m · sec ⁻³ · K ⁻¹
0.06292 · kg · m · sec ⁻³ · K ⁻¹
0.06788 · kg · m · sec ⁻³ · K ⁻¹
0.08631 · kg · m · sec ⁻³ · K ⁻¹

$$\lambda_{\text{mix}}(.0, 1000 \cdot K) = 6.64 \cdot 10^{-4} \cdot \frac{W}{\text{cm} \cdot K}$$

T02280"E99EE660

Define thermal conductivity of alumina and SS321

$$\text{Altc} = \begin{bmatrix} 83.71 \\ 224.898 \\ 255.842 \\ 132.727 \\ 25.9695 \end{bmatrix}$$

The parameter set Alt_c_n was determined from published values of the thermal conductivity. Ref: HCP

$\lambda_{\text{Al2O3}}(x)$ is the thermal conductivity function (of x with unit K) while λ_1 is its derivative w/r to temperature.

$$\lambda_{\text{Al2O3}}(x) := \sum_{n=0}^4 \text{Altc}_n \cdot \left(\frac{x}{1000 \cdot \text{K}} \right)^n \cdot \frac{\text{W}}{\text{m} \cdot \text{K}} \quad \lambda_1(x) := \sum_{n=1}^4 \frac{\text{Altc}_n}{1000 \cdot \text{K}} \cdot n \cdot \left(\frac{x}{1000 \cdot \text{K}} \right)^{n-1} \cdot \frac{\text{W}}{\text{m} \cdot \text{K}}$$

$$\text{S321tc} = \begin{bmatrix} 4.69312 \\ 4.9812 \\ -0.33357 \\ 0 \\ 0 \end{bmatrix}$$

The parameter set S321tc_n was determined from published values of the thermal conductivity. Ref: Handbook of Metals 8th Ed. Vol. 1 p. 423

$$\lambda_{\text{ss321}}(x) := \sum_{n=0}^4 \text{S321tc}_n \cdot \left(\frac{x}{1000 \cdot \text{K}} \right)^n \cdot \frac{\text{W}}{\text{m} \cdot \text{K}}$$

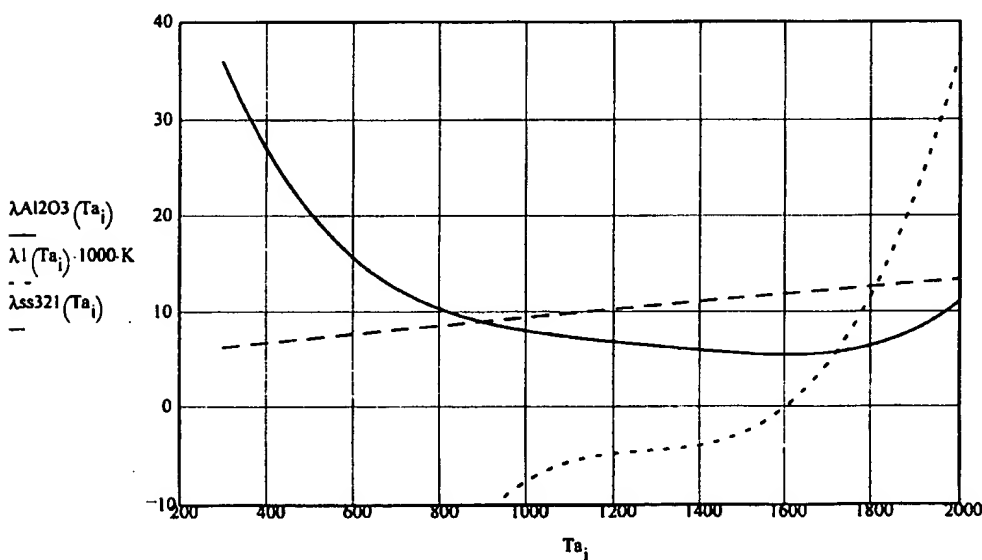
$$\lambda_{\text{ss321}}(1000 \cdot \text{K}) = 9.341 \cdot \frac{\text{W}}{\text{m} \cdot \text{K}}$$

$$\lambda_{\text{Al2O3}}(1000 \cdot \text{K}) = 7.897 \cdot \frac{\text{W}}{\text{m} \cdot \text{K}}$$

$$\lambda_1(1000 \cdot \text{K}) \cdot 1000 \cdot \text{K} = -7.517 \cdot \frac{\text{W}}{\text{m} \cdot \text{K}}$$

$$i := 30, 31 \dots 200$$

$$T_{a_i} := 10 \cdot i \cdot \text{K}$$



102280" E99EE660

$$x := 1500 \cdot K$$

$$x0 := \text{root}(\lambda 1(x), x)$$

$$x0 = 1.588 \cdot 10^3 K$$

$$\lambda_{ss321}(300 \cdot K) = 6.157 \cdot \frac{W}{m \cdot K}$$

$$0.003 \cdot \text{in} = 7.62 \cdot 10^{-3} \cdot \text{cm}$$

$$\lambda_{Al2O3}(300 \cdot K) = 0.359 \cdot \frac{W}{cm \cdot K}$$

$$\lambda_{Al2O3}(200 \cdot K) = 0.479 \cdot \frac{W}{cm \cdot K}$$

$$\lambda_{Al2O3}(800 \cdot K) = 0.102 \cdot \frac{W}{cm \cdot K}$$

$$\lambda_{Al2O3}(x0) = 0.054 \cdot \frac{W}{cm \cdot K}$$

Minimum thermal conductivity

Determine thermal conductivity of porous wall:

Ref: RHG - Handbook Chpt 6 for effective thermal conductivity including convection and radiative terms

$$\epsilon_{rad} := 0.6$$

$$\epsilon := 0.42$$

$$dp := 0.00005 \cdot \text{cm}$$

$$dp = 5 \cdot 10^{-7} \cdot \text{m}$$

$$\lambda_{wc}(x, T) := \lambda_{mix}(x, T) \cdot \left[0.0931 + 2 \cdot 0.9069 \cdot \left(\frac{\lambda_{Al2O3}(T)}{\lambda_{Al2O3}(T) - \lambda_{mix}(x, T)} \right)^2 \cdot \left(\ln \left(\frac{\lambda_{Al2O3}(T)}{\lambda_{mix}(x, T)} \right) - 1 \right) \right] \dots$$

$$+ 0.229 \cdot 10^{-6} \cdot \frac{W}{m^2 \cdot K^4} \cdot \epsilon \cdot dp \cdot \epsilon_{rad} \cdot T^3 \cdot \left[\epsilon + \frac{\left(0.229 \cdot 10^{-6} \cdot \frac{W}{m^2 \cdot K^4} \cdot \epsilon \cdot dp \cdot \epsilon_{rad} \cdot T^3 \right)}{\lambda_{Al2O3}(T)} + 1 \right]$$

$$\lambda_{wcnr}(x, T) := \lambda_{mix}(x, T) \cdot \left[0.0931 + 2 \cdot 0.9069 \cdot \left(\frac{\lambda_{Al2O3}(T)}{\lambda_{Al2O3}(T) - \lambda_{mix}(x, T)} \right)^2 \cdot \left(\ln \left(\frac{\lambda_{Al2O3}(T)}{\lambda_{mix}(x, T)} \right) - 1 \right) \right]$$

$$\lambda_{wc}(0.01, 1000 \cdot K) = 0.473 \cdot \frac{W}{m \cdot K}$$

$$\lambda_{wcnr}(0.01, 1000 \cdot K) = 0.473 \cdot \frac{W}{m \cdot K}$$

Radiation component negligible with such small particles in the washcoat

$$\lambda_{mix}(0.01, 1000 \cdot K) = 0.067 \cdot \frac{W}{m \cdot K}$$

$$\lambda_{Al2O3}(700 \cdot K) = 12.354 \cdot \frac{W}{m \cdot K}$$

$$\lambda_{ss321}(1000 \cdot K) = 9.341 \cdot \frac{W}{m \cdot K}$$

102280" E99EE660

$$\frac{\lambda_{Al_2O_3}(1000 \cdot K)}{\lambda_{mix}(0.01, 1000 \cdot K)} = 117.74$$

$$\frac{\lambda_{wc}(0.01, 1000 \cdot K)}{\lambda_{mix}(0.01, 1000 \cdot K)} = 7.046$$

The thermal conductivity of the wash coat is about 7 times greater at 1000K than the gas phase conductivity

$$\frac{\lambda_{wc}(0.01, 1000 \cdot K)}{\lambda_{ss321}(1000 \cdot K)} = 0.051$$

$$\frac{\frac{\lambda_{wc}(0.01, 1000 \cdot K)}{0.001 \cdot \text{cm}} + \frac{\lambda_{ss321}(1000 \cdot K)}{0.003 \cdot \text{in}}}{\frac{\lambda_{ss321}(1000 \cdot K)}{0.003 \cdot \text{in}}} = 1.386$$

The washcoat increases the thermal conductance of the wall by about 39%

$$\frac{\lambda_{ss321}(1000 \cdot K)}{\lambda_{mix}(0.01, 1000 \cdot K)} = 139.275$$

For a Nusselt no. of 2.976 ($d_{cell8} = 0.0961 \cdot \text{cm}$) for developed flow in the recuperator (full power) the mean heat transfer boundary layer thickness is much greater than either the SS321 wall thickness or the washcoat thickness.

$$\delta_{gprecup} := \frac{0.0961 \cdot \text{cm}}{2.976}$$

$$\delta_{gprecup} = 0.032 \cdot \text{cm}$$

$$h_{recavg}(T) := \frac{1}{\left(\frac{2}{\frac{\lambda_{mix}(0.01, T)}{\delta_{gprecup}}} \right) + \frac{1}{\frac{\lambda_{ss321}(1000 \cdot K)}{0.003 \cdot \text{in}}}}$$

Overall local heat transfer coefficient for the recuperator (assuming gas phase conductivities are about the same)

$$h_{recavgwc}(T) := \frac{1}{\left[\frac{1}{\frac{\lambda_{mix}(0.01, T)}{\delta_{gprecup} - \frac{2 \cdot 0.001 \cdot \text{cm}}{2.976}}} \right] + \left(\frac{1}{\frac{\lambda_{mix}(0.01, T)}{\delta_{gprecup}}} \right) + \left(\frac{1}{\frac{\lambda_{ss321}(1000 \cdot K)}{0.003 \cdot \text{in}}} \right) + \frac{\text{Effect of wash coat on heat transfer coefficient}}{\frac{\lambda_{wc}(0.01, T)}{0.001 \cdot \text{cm}}}}$$

$$h_{recavg}(1000 \cdot K) = 0.01038 \cdot \frac{W}{\text{cm}^2 \cdot K}$$

$$h_{recavgwc}(1000 \cdot K) = 0.01046 \cdot \frac{W}{\text{cm}^2 \cdot K}$$

The wash coat makes about 0.1% increase in heat transfer coefficient because of the slightly decreased cell size and greater thermal conductivity of the washcoat vs. gas phase.

102280" E99EE660